APPENDIX G
Lead and Feature Articles and Topical Reviews (2014 to date)

Article title	Author(s)	Journal	Issue	Citations (WoS)	Scopus	Altmetric	Views	Category	Access	Keywords	Review scores
Crystal structure refinement with SHELXL	G. M. Sheldrick	C	January 2015	42702	15852	34	64650	fe	Open	SHELXL; crystal structure refinement; X-ray and neutron diffraction; SHREDCIF	
The Cambridge Structural Database	C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward	B	April 2016	6579	6575	37	24665	fe	Open	Cambridge Structural Database; CIF archive; open data; crystal structure database	5.0 (5,5)
PLATON SQUEEZE: a tool for the calculation of the disordered solvent contribution to the calculated structure factors	A. L. Spek	C	January 2015	2895	2825	15	19453	fe		SQUEEZE; PLATON; embedded solvent; disorder	
Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix	D. Liebschner, P. V. Afonine, M. L. Baker, G. Bunkóczi, V. B. Chen, T. I. Croll, B. Hintze, L.-W. Hung, S. Jain, A. J. McCoy, N. W. Moriarty, R. D. Oeffner, B. K. Poon, M. G. Prisant, R. J. Read, J. S. Richardson, D. C. Richardson, M. D. Sammito, O. V. Sobolev, D. H. Stockwell, T. C. Terwilliger, A. G. Urzhumtsev, L. L. Videau, C. J. Williams and P. D. Adams	D	October 2019	2206	2651	52	19473	fe	Open	Phenix; automation; macromolecular crystallography; cryo-EM; X-rays; neutrons; diffraction; Python; cctbx; C++	5.0 (5)
Report on the sixth blind test of organic crystal structure prediction methods	A. M. Reilly, R. I. Cooper, C. S. Adjiman, S. Bhattacharya, A. D. Boese, J. G. Brandenburg, P. J. Bygrave, R. Bylsma, J. E. Campbell, R. Car, D. H. Case, R. Chadha, J. C. Cole, K. Cosburn, H. M. Cuppen, F. Curtis, G. M. Day, R. A. DiStasio Jr, A. Dzyabchenko, B. P. van Eijck, D. M. Elking, J. A. van den Ende, J. C. Facelli, M. B. Ferraro, L. Fusti-Molnar, C.-A. Gatsiou, T. S. Gee, R. de Gelder, L. M. Ghiringhelli, H. Goto, S. Grimme, R. Guo, D. W. M. Hofmann, J. Hoja, R. K. Hylton, L. Iuzzolino, W. Jankiewicz, D. T. de Jong, J. Kendrick, N. J. J. de Klerk, H.-Y. Ko, L. N. Kuleshova, X. Li, S. Lohani, F. J. J. Leusen, A. M. Lund, J. Lv, Y. Ma, N. Marom, A. E. Masunov, P. McCabe, D. P. McMahon, H. Meekes, M. P. Metz, A. J. Misquitta, S. Mohamed, B. Monserrat, R. J. Needs, M. A. Neumann, J. Nyman, S. Obata, H. Oberhofer, A. R. Oganov, A. M. Orendt, G. I. Pagola, C. C.	B	August 2016	418	419	37	27037	fe	Open	crystal structure prediction; polymorphism; lattice energies; Cambridge Structural Database	4.0 (4,4)

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	Pantelides, C. J. Pickard, R. Podeszwa, L. S. Price, S. L. Price, A. Pulido, M. G. Read, K. Reuter, E. Schneider, C. Schober, G. P. Shields, P. Singh, I. J. Sugden, K. Szalewicz, C. R. Taylor, A. Tkatchenko, M. E. Tuckerman, F. Vacarro, M. Vasileiadis, A. Vazquez-Mayagoitia, L. Vogt, Y. Wang, R. E. Watson, G. A. de Wijs, J. Yang, Q. Zhu and C. R. Groom										
Crystalline metal-organic frameworks (MOFs): synthesis, structure and function	C. Dey, T. Kundu, B. P. Biswal, A. Mallick and R. Banerjee	B	February 2014	234	261	7	33268	fe		metal-organic frameworks; crystal engineering; microporous materials; synthetic methods	
Serial femtosecond crystallography: the first five years	I. Schlichting	IUCrJ	March 2015	229	233	17	24452	fe	Open	serial femtosecond crystallography; SFX; X-ray lasers; FELs; time-resolved crystallography; microcrystals; radiation damage	
Advanced grazing-incidence techniques for modern soft-matter materials analysis	A. Hexemer and P. Müller-Buschbaum	IUCrJ	January 2015	183	188	2	21266	fe	Open	grazing-incidence techniques; GISAXS; GIWAXS; resonant soft X-ray scattering; GISANS; morphology; soft matter	4.0 (4)
EXAFS and XANES analysis of oxides at the nanoscale	A. Kuzmin and J. Chaboy	IUCrJ	November 2014	166	167	5	16205	fe	Open	EXAFS; XANES; oxide nanomaterials; nanocrystalline materials	4.0 (4)
XFELs for structure and dynamics in biology	J. C. H. Spence	IUCrJ	July 2017	119	125	19	21064	fe	Open	X-ray lasers; XFELs; biology; structure; dynamics	4.0 (5,4,3)
Supramolecular interactions in the solid state	G. Resnati, E. Boldyreva, P. Bombicz and M. Kawano	IUCrJ	November 2015	100	100	1	9415	fe	Open	intermolecular interactions; crystal engineering; self-assembly; halogen bonding; polymorphism; kinetic assembly; coordination polymers; non-ambient conditions; phase transitions	
NMR crystallography: structure and properties of materials from	D. L. Bryce	IUCrJ	July 2017	97	100	6	9066	tr	Open	Nuclear magnetic resonance; solid-state	4.0 (4,4)

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solid-state nuclear magnetic resonance observables										NMR; NMR crystallography; dynamics; noncovalent interactions	
Sub-atomic resolution X-ray crystallography and neutron crystallography: promise, challenges and potential	M. P. Blakeley, S. S. Hasnain and S. V. Antonyuk	IUCrJ	July 2015	95	92	16	14493	tr	Open	neutron; X-ray; hydrogen; proton; protonation states; radiation damage; redox biology; proton coupling; electron transfer; X-ray laser; XFEL	3.3 (5,4,1)
The HEPS project	Y. Jiao, G. Xu, X.-H. Cui, Z. Duan, Y.-Y. Guo, P. He, D.-H. Ji, J.-Y. Li, X.-Y. Li, C. Meng, Y.-M. Peng, S.-K. Tian, J.-Q. Wang, N. Wang, Y.-Y. Wei, H.-S. Xu, F. Yan, C.-H. Yu, Y.-L. Zhao and Q. Qin	JSR	November 2018	95	118	2	6792	fe	Open	High Energy Photon Source (HEPS); diffraction-limited storage ring; modified hybrid seven-bend achromat	3.0 (4,2)
Precession electron diffraction - a topical review	P. A. Midgley and A. S. Eggeman	IUCrJ	January 2015	91	104	2	16697	tr	Open	precession electron diffraction (PED); electron crystallography; electron techniques; electron-based structure analysis	4.0 (4,4)
PETRA IV: the ultralow-emittance source project at DESY	C. G. Schroer, I. Agapov, W. Brefeld, R. Brinkmann, Y.-C. Chae, H.-C. Chao, M. Eriksson, J. Keil, X. Nuel Gavaldà, R. Röhlsberger, O. H. Seeck, M. Sprung, M. Tischer, R. Wanzenberg and E. Weckert	JSR	September 2018	84	101	11	8701	fe	Open	PETRA IV; ultralow-emittance source; diffraction-limited storage ring	3.5 (4,3)
Structural studies of metal-organic frameworks under high pressure	S. C. McKellar and S. A. Moggach	B	December 2015	82	81	7	17792	fe	Free	high-pressure studies; MOFs; coordination polymers	3.5 (5,2)
MicroED data collection and processing	J. Hattne, F. E. Reyes, B. L. Nannenga, D. Shi, M. J. de la Cruz, A. G. W. Leslie and T. Gonen	A	July 2015	82	87	0	8589	fe	Open	MicroED; electron diffraction; crystallography; cryo-EM; nanocrystals	3.0 (4,2)
In-cell NMR: a topical review	E. Luchinat and L. Banci	IUCrJ	March 2017	81	86	26	12392	tr	Open	in-cell NMR; nuclear magnetic resonance; cellular structural biology; cellular environment; protein interactions	4.0 (5,3)
Crystallographic studies of gas sorption in metal-organic frameworks	E. J. Carrington, I. J. Vitórica-Yrezábal and L. Brammer	B	June 2014	80	81	1	9769	fe	Open	metal-organic frameworks; gas sorption; framework flexibility	

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Compound focusing mirror and X-ray waveguide optics for coherent imaging and nano-diffraction	T. Salditt, M. Osterhoff, M. Krenkel, R. N. Wilke, M. Priebe, M. Bartels, S. Kalbfleisch and M. Sprung	JSR	July 2015	69	68	1	5349	fe	Free	coherent imaging; nano-diffraction; waveguides; holography	4.0 (4)
Quasicrystals: What do we know? What do we want to know? What can we know?	W. Steurer	A	January 2018	67	69	32	9767	tr	Open	quasicrystals; structure analysis; higher-dimensional crystallography; stability of quasicrystals; quasicrystal growth	3.5 (4,3)
Lytic polysaccharide monooxygenases: a crystallographer's view on a new class of biomass-degrading enzymes	K. E. H. Frandsen and L. Lo Leggio	IUCrJ	November 2016	66	68	9	7724	tr	Open	lytic polysaccharide monooxygenases; carbohydrate-modifying enzymes; metalloproteins; copper enzymes; biomass degradation	
FemtoSpeX: a versatile optical pump-soft X-ray probe facility with 100 fs X-ray pulses of variable polarization	K. Holldack, J. Bahrdt, A. Balzer, U. Bovensiepen, M. Brzhezinskaya, A. Erko, A. Eschenlohr, R. Follath, A. Firsov, W. Frentrup, L. Le Guyader, T. Kachel, P. Kuske, R. Mitzner, R. Müller, N. Pontius, T. Quast, I. Radu, J.-S. Schmidt, C. Schüßler-Langeheine, M. Sperling, C. Stamm, C. Trabant and A. Föhlisch	JSR	September 2014	66	69	2	9282	la	Free	femtosecond X-ray pulses; storage ring; elliptical undulators; slicing; diffractive optics; time-resolved X-ray spectroscopy; ultrafast science	3.0 (3)
Metadynamics studies of crystal nucleation	F. Giberti, M. Salvalaglio and M. Parrinello	IUCrJ	March 2015	62	68	2	15890	fe	Open	crystallization; nucleation; molecular modelling; enhanced sampling; metadynamics	3.0 (4,2)
X-ray imaging detectors for synchrotron and XFEL sources	T. Hatsui and H. Graafsma	IUCrJ	May 2015	59	63	5	14338	fe	Open	X-ray imaging detectors; hybrid detectors; monolithic detectors; recent detector developments	3.0 (3,3)
Bond-length distributions for ions bonded to oxygen: results for the transition metals and quantification of the factors underlying bond-length variation in inorganic solids	O. C. Gagné and F. C. Hawthorne	IUCrJ	July 2020	58	57	41	8626	la	Open	bond-length variation; bond-topological effects; vibronic mixing; pseudo Jahn-Teller effect; materials design	4.5 (5,4)
Three-dimensional electron diffraction as a complementary technique to powder X-ray	Y. Yun, X. Zou, S. Hovmöller and W. Wan	IUCrJ	March 2015	58	54	3	12873	fe	Open	three-dimensional electron diffraction; powder X-ray diffraction;	3.0 (3,3)

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diffraction for phase identification and structure solution of powders										phase identification; structure determination	
Towards understanding π-stacking interactions between non-aromatic rings	K. Molčanov and B. Kojić-Prodić	IUCrJ	March 2019	55	55	3	10061	tr	Open	π-stacking interactions; non-aromatic rings; multicentric bonding; charge	4.0 (4,4)
Progress in small-angle scattering from biological solutions at high-brilliance synchrotrons	A. T. Tuukkanen, A. Spilotros and D. I. Svergun	IUCrJ	September 2017	52	55	15	9508	tr	Open	small-angle X-ray scattering; structural modelling; time-resolved SAXS	3.3 (4,3,3)
Commissioning and first-year operational results of the MAX IV 3 GeV ring	P. F. Tavares, E. Al-Dmour, Å. Andersson, F. Cullinan, B. N. Jensen, D. Olsson, D. K. Olsson, M. Sjöström, H. Tarawneh, S. Thorin and A. Vorozhtsov	JSR	September 2018	52	55	5	6146	fe	Open	storage ring; synchrotron light source; multibend achromat; MAX IV	4.5 (5,4)
Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry	T. L. Blundell	IUCrJ	July 2017	51	60	23	17520	fe	Open	protein structure; protein crystallography; fragment-based structure-guided drug discovery; disease; cancer	4.0 (4)
Native SAD is maturing	J. P. Rose, B.-C. Wang and M. S. Weiss	IUCrJ	July 2015	47	41	4	11372	fe	Open	native SAD; sulfur SAD; accurate data collection; data multiplicity; radiation damage; new instruments; new data-scaling techniques	4.0 (4,4)
Crystallography of metal-organic frameworks	F. Gándara and T. D. Bennett	IUCrJ	November 2014	46	50	5	19983	fe	Open	MOFs; non-ambient crystallography; crystal growth	5.0 (5,5)
Macromolecular ab initio phasing enforcing secondary and tertiary structure	C. Millán, M. Sammito and I. Usón	IUCrJ	January 2015	46	36	2	11175	fe	Open	ab initio phasing; α-helices; macromolecular structure; ARCIMBOLDO	3.0 (4,2)
Protein microcrystallography using synchrotron radiation	M. Yamamoto, K. Hirata, K. Yamashita, K. Hasegawa, G. Ueno, H. Ago and T. Kumasaka	IUCrJ	September 2017	45	40	13	7146	tr	Open	protein microcrystallography; multi-point data collection; multi-crystal data collection; serial synchrotron crystallography	3.0 (4,3,2)
Aperiodic crystals and	T. Janssen and A. Janner	B	August	45	46	3	10157	la	Free	aperiodic crystals;	4.0

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superspace concepts			2014							superspace concepts; lattice periodicity	(5,3)
Neutron scattering in the biological sciences: progress and prospects	R. Ashkar, H. Bilheux, H. Bordallo, R. Briber, D. J. E. Callaway, X. Cheng, X.-Q. Chu, J. E. Curtis, M. Dadmun, P. Fenimore, D. Fushman, F. Gabel, K. Gupta, F. Herberle, F. Heinrich, L. Hong, J. Katsaras, Z. Kelman, E. Kharlampieva, G. R. Kneller, A. Kovalevsky, S. Krueger, P. Langan, R. Lieberman, Y. Liu, M. Losche, E. Lyman, Y. Mao, J. Marino, C. Mattos, F. Meilleur, P. Moody, J. D. Nickels, W. B. O'Dell, H. O'Neill, U. Perez-Salas, J. Peters, L. Petridis, A. P. Sokolov, C. Stanley, N. Wagner, M. Weinrich, K. Weiss, T. Wymore, Y. Zhang and J. C. Smith	D	December 2018	43	41	7	4118	la		neutron scattering; biological systems; structure and dynamics	4.5 (5,4)
CM01: a facility for cryo-electron microscopy at the European Synchrotron	E. Kandiah, T. Giraud, A. de Maria Antolinos, F. Dobias, G. Effantin, D. Flot, M. Hons, G. Schoehn, J. Susini, O. Svensson, G. A. Leonard and C. Mueller-Dieckmann	D	June 2019	43	51	26	5050	fe	Open	cryo-TEM; ESRF; PSB; cryo-EM platform; CM01	3.0 (3,3,3)
The potential of future light sources to explore the structure and function of matter	E. Weckert	IUCrJ	March 2015	42	47	2	14922	fe	Open	synchrotron radiation; future light sources; FELs; coherent radiation	5.0 (5,5)
Making crystals with a purpose; a journey in crystal engineering at the University of Bologna	D. Braga, F. Grepioni, L. Maini and S. d'Agostino	IUCrJ	July 2017	40	41	6	6679	tr	Open	cocrystals; solid solutions; polymorphism; luminescence; chirality	4.0 (4,4)
Hexagonal $RMnO_3$: a model system for two-dimensional triangular lattice antiferromagnets	H. Sim, J. Oh, J. Jeong, M. D. Le and J.-G. Park	B	February 2016	39	43	27	5454	fe	Free	multiferroic materials; ferroelectricity; magnetic structures; magnetic frustration; spin-lattice coupling	4.0 (4)
Structure-directing effects of ionic liquids in the ionothermal synthesis of metal-organic frameworks	T. P. Vaid, S. P. Kelley and R. D. Rogers	IUCrJ	July 2017	39	42	1	7019	tr	Open	metal-organic framework; MOF; ionic liquid; ionothermal synthesis; template	4.5 (5,4)
The solvent component of macromolecular crystals	C. X. Weichenberger, P. V. Afonine, K. Kantardjieff and B. Rupp	D	May 2015	37	38	36	9762	fe		macromolecular crystals; solvent content; bulk solvent; ordered solvent	4.0 (5,4,3)
Cryo-electron microscopy and X-ray crystallography: complementary approaches to structural biology and drug discovery	C. Vénien-Bryan, Z. Li, L. Vuillard and J. A. Boutin	F	April 2017	36	42	29	10521	tr	Open	cryo-electron microscopy; cryo-EM; structural biology; high resolution; conformational	2.7 (4,3,1)

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										variability; drug discovery	
High pressure and multiferroics materials: a happy marriage	E. Gilioli and L. Ehm	IUCrJ	November 2014	35	41	1	9694	fe	Open	high pressure; multiferroics; materials science	4.0 (4)
The first X-ray diffraction measurements on Mars	D. Bish, D. Blake, D. Vaniman, P. Sarrazin, T. Bristow, C. Achilles, P. Dera, S. Chipera, J. Crisp, R. T. Downs, J. Farmer, M. Gailhanou, D. Ming, J. M. Morookian, R. Morris, S. Morrison, E. Rampe, A. Treiman and A. Yen	IUCrJ	November 2014	35	35	60	17615	fe	Open	X-ray diffraction; Mars; extraterrestrial mineralogy; Curiosity rover	5.0 (5)
Perspectives on Li and transition metal fluoride phosphates as cathode materials for a new generation of Li-ion batteries	E. V. Antipov, N. R. Khasanova and S. S. Fedotov	IUCrJ	January 2015	34	35	4	9302	fe	Open	Li-ion batteries; cathode materials; transition metal fluoride phosphates; structure-property relationships	4.0 (4,4)
Contemporary X-ray electron-density studies using synchrotron radiation	M. R. V. Jørgensen, V. R. Hathwar, N. Bindzus, N. Wahlberg, Y.-S. Chen, J. Overgaard and B. B. Iversen	IUCrJ	September 2014	33	32	2	10041	fe	Open	electron-density studies; synchrotron radiation; X-ray diffraction	4.0 (4,4,4)
SLS-2 - the upgrade of the Swiss Light Source	A. Streun, T. Garvey, L. Rivkin, V. Schlott, T. Schmidt, P. Willmott and A. Wrulich	JSR	May 2018	33	42	8	5783	fe	Open	synchrotron radiation facility; electron storage ring; low-emittance lattice; undulator; imaging; molecular biology; X-ray spectroscopy	5.0 (5)
An overview of comparative modelling and resources dedicated to large-scale modelling of genome sequences	S. D. Lam, S. Das, I. Sillitoe and C. Orengo	D	August 2017	32	37	8	6418	tr	Open	protein structure prediction; template-based modelling; comparative modelling; template selection	3.5 (5,2)
Real-time powder diffraction studies of energy materials under non-equilibrium conditions	V. K. Peterson, J. E. Auckett and W.-K. Pang	IUCrJ	September 2017	31	32	3	6530	tr	Open	real-time studies; operando studies; powder diffraction; functional materials; energy materials	3.5 (4,3)
Structural chemistry of layered lead halide perovskites containing single octahedral layers	J. A. McNulty and P. Lightfoot	IUCrJ	July 2021	31	0	7	5014	la	Open	layered perovskites; symmetry mode analysis; hybrid materials	4.0 (4,4)
Precise implications for real-space pair distribution function	D. Olds, C. N. Saunders, M. Peters, T. Proffen, J. Neuefeind and K. Page	A	July 2018	30	28	4	5300	fe		total scattering; pair distribution function;	2.0 (2)

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modeling of effects intrinsic to modern time-of-flight neutron diffractometers										instrument resolution function; time-of-flight peak shapes	
Automated electron diffraction tomography - development and applications	U. Kolb, Y. Krysiak and S. Plana-Ruiz	B	August 2019	30	32	4	6710	la	Open	electron diffraction tomography; single-crystal structure analysis; disorder analysis; nanomaterials; electron crystallography	3.0 (3)
Raw diffraction data preservation and reuse: overview, update on practicalities and metadata requirements	L. M. J. Kroon-Batenburg, J. R. Helliwell, B. McMahon and T. C. Terwilliger	IUCrJ	January 2017	30	28	48	10943	tr	Open	raw diffraction data; data archiving; metadata descriptors for raw data; diversity of crystallographic instrumentation	4.5 (5,4)
Electronic materials with a wide band gap: recent developments	D. Klimm	IUCrJ	September 2014	29	35	3	16143	fe	Open	electronic materials; wide band gap materials; semiconductors; silicon; germanium	4.0 (4,4)
Diffuse scattering and partial disorder in complex structures	T. R. Welberry and D. J. Goossens	IUCrJ	November 2014	29	30	1	14570	fe	Open	single-crystal diffuse scattering; disorder; synchrotron light sources	3.0 (3)
Applications of contact predictions to structural biology	F. Simkovic, S. Ovchinnikov, D. Baker and D. J. Rigden	IUCrJ	May 2017	28	32	6	11034	tr	Open	evolutionary covariance; predicted contacts; NMR distance restraints; X-ray crystallography; structural bioinformatics	4.0 (4)
Covering complete proteomes with X-ray structures: a current snapshot	M. J. Mizianty, X. Fan, J. Yan, E. Chalmers, C. Woloschuk, A. Joachimiak and L. Kurgan	D	November 2014	27	29	34	9044	fe	Open	crystallization propensity; proteome coverage; fDETECT	4.0 (4)
Synchrotron radiation macromolecular crystallography: science and spin-offs	J. R. Helliwell and E. P. Mitchell	IUCrJ	March 2015	27	29	11	12536	tr	Open	automation; microcrystals; storage-ring upgrades; X-ray lasers; neutrons; industrial and commercial access; expanding wavelength range; time-resolved studies; dynamics; diffuse scattering; room-temperature studies; raw data	2.5 (4,1)

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Advanced electron crystallography through model-based imaging	S. Van Aert, A. De Backer, G. T. Martinez, A. J. den Dekker, D. Van Dyck, S. Bals and G. Van Tendeloo	IUCrJ	January 2016	27	30	2	8687	fe	Open	transmission electron microscopy; quantitative analysis; statistical parameter estimation; experimental design; structure refinement	2.5 (4,1)
A structural overview of the zinc transporters in the cation diffusion facilitator family	C. A. Cotrim, R. J. Jarrott, J. L. Martin and D. Drew	D	April 2019	27	32	13	5280	tr	Open	cation diffusion facilitator; membrane proteins; zinc transporter	4.0 (4,4)
Contributions of charge-density research to medicinal chemistry	B. Dittrich and C. F. Matta	IUCrJ	November 2014	26	28	2	12068	fe	Open	charge-density research; medicinal chemistry; drug design; invariom; Hansen-Coppens multipole model; quantum theory of atoms in molecules	3.0 (3,3,3)
Copper minerals from volcanic exhalations - a unique family of natural compounds: crystal-chemical review	I. V. Pekov, N. V. Zubkova and D. Y. Pushcharovsky	B	December 2018	26	30	2	435	tr		copper minerals; crystal chemistry; volcanic exhalations; fumarole minerals; oxocentred tetrahedra	3.5 (4,3)
Pressure effects on lipids and bio-membrane assemblies	N. J. Brooks	IUCrJ	November 2014	26	26	244	9534	fe	Open	biological membranes; lipids; bilayers; lipid-protein assemblies; high-pressure studies	2.0 (3,1)
Modelling the experimental electron density: only the synergy of various approaches can tackle the new challenges	P. Macchi, J.-M. Gillet, F. Taulelle, J. Campo, N. Claiser and C. Lecomte	IUCrJ	July 2015	25	26	2	8673	fe	Open	charge density; spin density; momentum density	3.5 (4,3)
Superspace crystallography: a key to the chemistry and properties	C. B. Pinheiro and A. M. Abakumov	IUCrJ	January 2015	24	24	3	17052	tr	Open	superspace crystallography; modulated structure; incommensurate modulation; chemistry	3.0 (3,3)
Multiple-scale structures: from Faraday waves to soft-matter quasicrystals	S. Savitz, M. Babadi and R. Lifshitz	IUCrJ	May 2018	24	23	2	4965	tr	Open	quasicrystals; soft matter; pattern formation	4.5 (5,4)
Lab in a DAC - high-pressure crystal chemistry in a diamond-anvil cell	A. Katrusiak	B	December 2019	24	25	8	12564	la		extreme conditions; diamond-anvil cell; thermodynamic transformations; chemical reactions	4.0 (4)

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The `quasi-mosaic' effect in crystals and its applications in modern physics	R. Camattari, V. Guidi, V. Bellucci and A. Mazzolari	JAC	August 2015	23	22	1	4215	fe		quasi-mosaicity; hard X-ray focalization; charged-particle beam steering	3.3 (4,3,3)
Computation in electron microscopy	E. J. Kirkland	A	January 2016	23	23	6	8451	la	Free	high-resolution transmission electron microscopy; HRTEM; multislice method; exit-wave reconstruction; deconvolution	3.0 (4,2)
Functional materials analysis using in situ and in operando X-ray and neutron scattering	V. K. Peterson and C. M. Papadakis	IUCrJ	March 2015	23	25	1	12602	tr	Open	functional materials; X-ray scattering; neutron scattering; materials characterization	3.0 (3,3)
Aperiodic crystals and beyond	U. Grimm	B	June 2015	22	21	11	9812	fe	Free	aperiodic crystals; incommensurate structures; crystalline order; pattern theory; mathematical diffraction	4.0 (5,3)
Fifteen years of the Protein Crystallography Station: the coming of age of macromolecular neutron crystallography	J. C.-H. Chen and C. J. Unkefer	IUCrJ	January 2017	22	20	8	7515	fe	Open	neutron crystallography; Protein Crystallography Station; Los Alamos Neutron Scattering Center; H atoms; enzyme mechanisms	3.0 (3,3,3)
Recent advances of polyoxometalate-catalyzed selective oxidation based on structural classification	Q. Chen, C. Shen and L. He	C	November 2018	22	24	2	4485	fe		polyoxometalate; POM; selective oxidation; catalytic activity	3.5 (4,3)
Deformable elastic network refinement for low-resolution macromolecular crystallography	G. F. Schröder, M. Levitt and A. T. Brunger	D	September 2014	22	22	56	7835	fe	Open	deformable elastic network refinement; low resolution	3.0 (4,2)
Protein structure prediction by AlphaFold2: are attention and symmetries all you need?	N. Bouatta, P. Sorger and M. AlQuraishi	D	August 2021	22	26	43	31622	fe	Open	AlphaFold2; protein structure prediction; CASP14	
Source Function applied to experimental densities reveals subtle electron-delocalization effects and appraises their transferability properties in crystals	C. Gatti, G. Saleh and L. Lo Presti	B	April 2016	21	23	48	5322	fe	Free	Source Function; electron delocalization; chemical transferability; chemical bonding; X-ray derived electron density	4.5 (5,4)
Beyond simple small-angle X-	W. Bras, S. Koizumi and N. J. Terrill	IUCrJ	November	21	22	1	10590	fe	Open	SAXS; WAXS; SANS;	4.0

Article title	Author(s)	Journal	Issue	Citations (WoS)	Scopus	Altmetric	Views	Category	Access	Keywords	Review scores
ray scattering: developments in online complementary techniques and sample environments			2014							complementary techniques; sample environment	(4,4)
The science is in the data	J. R. Helliwell, B. McMahon, J. M. Guss and L. M. J. Kroon-Batenburg	IUCrJ	November 2017	20	21	20	7358	tr	Open	raw diffraction data; sharing raw data and its reuse; open science; education; crystallographic science case studies	2.0 (2)
A strenuous experimental journey searching for spectroscopic evidence of a bridging nickel-iron-hydride in [NiFe] hydrogenase	H. Wang, Y. Yoda, H. Ogata, Y. Tanaka and W. Lubitz	JSR	November 2015	20	20	0	4332	fe	Free	nuclear resonance vibrational spectroscopy; NRVS; ultra-weak signal; [NiFe] hydrogenase; Ni-R; Ni-H-Fe wag mode; iron hydride	3.0 (3)
Structure and function of dioxygenases in histone demethylation and DNA/RNA demethylation	C. Dong, H. Zhang, C. Xu, C. H. Arrowsmith and J. Min	IUCrJ	November 2014	20	23	1	10752	fe	Open	dioxygenases; histone demethylation; DNA/RNA demethylation; N6-methyladenosine; ALKBH5	5.0 (5)
Understanding geology through crystal engineering: coordination complexes, coordination polymers and metal-organic frameworks as minerals	I. Huskić and T. Friščić	B	December 2018	19	17	8	5695	fe		organic minerals; crystal engineering; metal-organic frameworks; MOFs; coordination polymers; hydrogen bonds; cocrystals	5.0 (5,5)
A survey of interactions in crystal structures of pyrazine-based compounds	F. Taghipour and M. Mirzaei	C	March 2019	19	18	1	3861	fe		pyrazine; magnetic properties; polyoxometalates; multinuclear; hydrogen bonding; metal-organic frameworks; POM; POMOF; MOF	2.0 (3,2,1)
Charge density and optical properties of multicomponent crystals containing active pharmaceutical ingredients or their analogues	M. Gryl	B	August 2015	17	13	0	6133	fe	Free	crystal engineering; active pharmaceutical ingredients; charge density studies; optical properties; ab initio calculations	3.5 (5,2)
Probing droplets on	A. Accardo, E. Di Fabrizio, T. Limongi, G.	JSR	July 2014	17	17	2	4522	fe	Open	superhydrophobic	

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superhydrophobic surfaces by synchrotron radiation scattering techniques	Marinaro and C. Riekel									surface; nanotechnology; biological matter; synchrotron radiation micro- and nanodiffraction	
Spin ballet for sweet encounters: saturation-transfer difference NMR and X-ray crystallography complement each other in the elucidation of protein-glycan interactions	B. S. Blaum, U. Neu, T. Peters and T. Stehle	F	August 2018	17	19	4	3314	tr	Open	saturation-transfer difference NMR; STD-NMR; polyomavirus; carbohydrates; lectins; structural biology	2.5 (4,1)
Visualization of biological macromolecules at near-atomic resolution: cryo-electron microscopy comes of age	A. K. Mitra	F	January 2019	17	3	8	3040	tr		cryo-EM; single-particle analysis; three-dimensional reconstruction; phase plates; direct detectors	4.0 (5,3)
`NMR Crystallization': in-situ NMR techniques for time-resolved monitoring of crystallization processes	K. D. M. Harris, C. E. Hughes, P. A. Williams and G. R. Edwards-Gau	C	March 2017	16	15	1	780	tr		NMR crystallography; in-situ NMR; CLASSIC NMR; time-resolved; crystallization processes	3.0 (3,3)
Topological features in crystal structures: a quotient graph assisted analysis of underlying nets and their embeddings	J.-G. Eon	A	May 2016	16	15	0	1103	la		crystal topology; labelled quotient graphs; ring analysis; building blocks	3.5 (4,3)
Synchrotron X-ray footprinting as a method to visualize water in proteins	S. Gupta, J. Feng, L. J. G. Chan, C. J. Petzold and C. Y. Ralston	JSR	September 2016	16	18	5	5355	fe	Free	bound water; hydroxyl radical labeling; mass spectrometry; protein conformation; protein modification	
Why direct and post-refinement determinations of absolute structure may give different results	D. J. Watkin and R. I. Cooper	B	October 2016	16	15	26	6669	fe	Free	absolute structure determination; Flack parameter; refinement; software; problem structures	4.0 (4,4)
Microfluidic devices for small-angle neutron scattering	C. G. Lopez, T. Watanabe, M. Adamo, A. Martel, L. Porcar and J. T. Cabral	JAC	June 2018	15	15	2	5169	fe		microfluidic devices; small-angle neutron scattering; lab-on-a-chip; closed-face polymer photolithography	2.0 (3,1)
The expanding toolkit for structural biology: synchrotrons, X-ray lasers and cryoEM	S. P. Muench, S. V. Antonyuk and S. S. Hasnain	IUCrJ	March 2019	15	17	15	6739	tr	Open	synchrotron crystallography; serial femtosecond	2.0 (3,1)

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										crystallography; cryoEM; MSOX	
Structural and biophysical aspects of l-asparaginases: a growing family with amazing diversity	J. I. Loch and M. Jaskolski	IUCrJ	July 2021	15	0	1	3575	fe	Open	leukemia; l-asparaginases; amidohydrolases; catalytic mechanism; active site; nucleophiles	4.0 (4)
The many flavours of halogen bonds - message from experimental electron density and Raman spectroscopy	R. Wang, J. George, S. K. Potts, M. Kremer, R. Dronskowski and U. Englert	C	September 2019	15	16	6	3414	fe	Open	halogen bonds; experimental electron density; AIM analysis; crystal engineering; crystal structure; Raman spectroscopy	4.3 (5,4,4)
Industrial cryo-EM facility setup and management	K. Sader, R. Matadeen, P. Castro Hartmann, T. Halsan and C. Schlichten	D	April 2020	15	18	14	8019	fe	Open	cryo-EM; facility setup; facility management; industry	3.0 (4,2)
Nanocrystalline materials: recent advances in crystallographic characterization techniques	E. Ringe	IUCrJ	November 2014	15	18	2	9236	fe	Open	nanocrystalline materials; plasmonics; shape prediction models	3.0 (4,2)
Viruses and viral proteins	N. Verdaguer, D. Ferrero and M. R. Murthy	IUCrJ	November 2014	15	17	4	14057	fe	Open	bacteriophages; genome delivery; fusion proteins; RNA-dependent RNA polymerases; viral proteases; viral receptors; viruses	4.0 (4)
High-pressure crystallography of periodic and aperiodic crystals	C. Hejny and V. S. Minkov	IUCrJ	March 2015	14	11	2	13260	fe	Open	high-pressure crystallography; periodic crystals; aperiodic crystals; incommensurate modulation	2.5 (3,2)
Application of synchrotron through-the-substrate microdiffraction to crystals in polished thin sections	J. Rius, O. Vallcorba, C. Frontera, I. Peral, A. Crespi and C. Miravitlles	IUCrJ	July 2015	14	12	3	7499	fe	Open	tts-μXRD; polished thin sections; crystal microvolume; Patterson function direct methods; δ recycling; synchrotron radiation; two-dimensional frame merging; multicrystal merging; structure solution	3.0 (3,3)
A perspective on structural and	E. Lira-Navarrete and R. Hurtado-Guerrero	F	August	14	14	4	2902	tr	Open	O-fucosylation; protein	4.0

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mechanistic aspects of protein O-fucosylation			2018							O-fucosyltransferases; epidermal growth factor-like repeats; EGF repeats; thrombospondin type I repeats; TSRs; enzyme mechanisms; GDP-fucose	(4,4)
A crystallographic excursion in the extraordinary world of minerals: the case of Cu- and Ag-rich sulfosalts	L. Bindi and C. Biagioni	B	December 2018	14	13	1	368	tr		copper; silver; sulfosalts; crystal structure; ionic conductivity; minerals	3.5 (5,2)
What is the structural chemistry of the living organism at its temperature and pressure?	J. R. Helliwell	D	February 2020	14	13	10	4020	fe	Open	structural biology; X-rays; neutrons; electrons	4.5 (5,4)
New methods in time-resolved Laue pump-probe crystallography at synchrotron sources	P. Coppens and B. Fournier	JSR	March 2015	14	16	1	7834	la	Free	photocrystallography; pink-Laue; orientation matrix determination; spot integration; multicrystal data sets	3.5 (4,3)
Advances in mass spectrometry based strategies to study receptor tyrosine kinases	S. Vyse, H. Desmond and P. H. Huang	IUCrJ	March 2017	13	13	4	6552	tr	Open	receptor tyrosine kinase; mass spectrometry; phosphoproteomics; signal transduction; cancer	3.0 (4,2)
The data universe of structural biology	H. M. Berman, B. Vallat and C. L. Lawson	IUCrJ	July 2020	13	17	7	4833	tr	Open	Protein Data Bank; structural biology; X-ray crystallography; data resources; data standards	4.0 (4,4)
Solid-state NMR and short-range order in crystalline oxides and silicates: a new tool in paramagnetic resonances	J. F. Stebbins, R. J. McCarty and A. C. Palke	C	March 2017	13	15	1	632	tr		nuclear magnetic resonance; solid-state NMR; SSNMR; paramagnetic shift; contact shift; silicates; oxides; transition metals; rare earth cations; crystal structure; geosciences	4.0 (4)
Synergy between transmission electron microscopy and powder diffraction: application to modulated structures	D. Batuk, M. Batuk, A. M. Abakumov and J. Hadermann	B	April 2015	13	13	33	6530	fe	Free	transmission electron microscopy; powder diffraction; anion-deficient perovskites; modulated structures	3.0 (3,3,3)
Structural dynamics: review of time-resolved cryo-EM	M.-E. Mäeots and R. I. Enchev	D	August 2022	13	15	23	6544	tr	Open	cryo-EM; time-resolved cryo-EM; sample	3.7 (4,4,3)

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										preparation; structural biology; structural dynamics	
Pressure-induced structural phase transformation in cobalt(II) dicyanamide	A. A. Yakovenko, K. W. Chapman and G. J. Halder	B	June 2015	12	14	55	5129	fe	Free	high pressure; magnetic molecular framework material; MOFs	4.0 (4,4)
A modulation wave approach to the order hidden in disorder	R. Withers	IUCrJ	January 2015	12	14	1	6115	fe	Open	modulation wave approach; ordered `disorder'; crystalline structure; long-range order; short-range order	4.0 (4,4)
Recent advances in isopolyoxotungstates and their derivatives	Y.-J. Liu, M.-T. Jin, L.-J. Chen and J.-W. Zhao	C	November 2018	12	13	2	2961	fe		polyoxometalate; isopolyoxotungstate; synthesis; structure; crystal structure	4.0 (4)
The atacamite family of minerals - a testbed for quantum spin liquids	T. Malcherek, M. D. Welch and P. A. Williams	B	December 2018	12	12	2	762	tr		Jahn-Teller distortion; spin liquid; geometric frustration; herbertsmithite; paratacamite; clinoatacamite	4.0 (4,4)
Structure solution and refinement of metal-ion battery cathode materials using electron diffraction tomography	J. Hadermann and A. M. Abakumov	B	August 2019	12	12		1071	fe		electron diffraction tomography; metal ion; lithium; battery; crystal structure	3.5 (4,3)
Reconciling the regulatory role of Munc18 proteins in SNARE-complex assembly	A. Rehman, J. K. Archbold, S.-H. Hu, S. J. Norwood, B. M. Collins and J. L. Martin	IUCrJ	November 2014	12	15	2	7183	fe	Open	SM proteins; SNARE proteins; syntaxin; Munc18; membrane trafficking	4.0 (4)
A simple graphical method to pinpoint local pseudosymmetries in Z′ > 1 cases	R. Baggio	C	July 2019	12	12	6	1310	fe		pseudosymmetry; ADDSYM; local symmetry; visual method	4.0 (5,3)
In situ electrochemical synchrotron radiation for Li-ion batteries	T. Alemu and F.-M. Wang	JSR	January 2018	11	10	1	3622	tr		in situ; synchrotron radiation; Li-ion battery; X-ray diffraction spectroscopy; transmission X-ray microscopy; X-ray absorption spectroscopy; solid electrolyte interphase	3.0 (3)

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Observing structural reorientations at solvent-nanoparticle interfaces by X-ray diffraction - putting water in the spotlight	M. Zobel	A	November 2016	11	14	1	853	la		solvent-nanoparticle interfaces; solvent restructuring; hydration shell; liquid structure; pair distribution function	4.0 (4)
Single-crystal-to-single-crystal transformations triggered by dehydration in polyoxometalate-based compounds	S. Reinoso, B. Artetxe and J. M. Gutiérrez-Zorrilla	C	November 2018	11	12	3	4502	fe		polyoxometalate; POM; crystal-to-crystal transitions; dynamic behaviour; robust frameworks; crystal engineering	4.0 (5,3)
Cryogenic coherent X-ray diffraction imaging of biological samples at SACLA: a correlative approach with cryo-electron and light microscopy	Y. Takayama and K. Yonekura	A	March 2016	11	15	1	4923	fe		coherent X-ray diffraction imaging; X-ray free-electron lasers; frozen-hydrated non-crystalline samples; structural analysis; correlative microscopy	4.0 (4,4)
Investigating increasingly complex macromolecular systems with small-angle X-ray scattering	B. Vestergaard and Z. Sayers	IUCrJ	November 2014	11	13	1	6294	fe	Open	biological solution small-angle X-ray scattering (BioSAXS); synchrotron radiation; beamlines; structural complexity; biostructural research	3.0 (3,3)
Brightness of synchrotron radiation from undulators and bending magnets	G. Geloni, V. Kocharyan and E. Saldin	JSR	March 2015	11	11	2	7049	la	Free	brightness; Wigner distribution; undulator radiation; bending magnet radiation	
Combining X-rays, neutrons and electrons, and NMR, for precision and accuracy in structure-function studies	J. R. Helliwell	A	May 2021	10	7	14	4054	la	Open	X-rays; neutrons; electrons; NMR; structure and function	4.5 (5,4)
Mean bond-length variations in crystals for ions bonded to oxygen	O. C. Gagné and F. C. Hawthorne	B	December 2017	10	10	1	3256	la		bond length; coordination number; distortion; electronegativity; ionization energy; structural strain; ionic radius; oxide; oxysalt	3.0 (5,1)
Data to knowledge: how to get meaning from your result	H. M. Berman, M. J. Gabanyi, C. R. Groom, J. E. Johnson, G. N. Murshudov, R. A. Nicholls, V. Reddy, T. Schwede, M. D. Zimmerman, J. Westbrook and W. Minor	IUCrJ	January 2015	10	10	3	14982	fe	Open	meaning from data; big data; databases; knowledge bases; data deposition	2.5 (4,1)

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Upscaling X-ray nanoimaging to macroscopic specimens	M. Du, Z. Di, D. Gürsoy, R. P. Xian, Y. Kozorovitskiy and C. Jacobsen	JAC	April 2021	10	11	1	3767	la	Open	X-ray microscopy; phase contrast X-ray imaging	3.0 (3)
A survey of the structural models proposed for $PbZr_{1-x}Ti_xO_3$ using mode analysis	B. Kocsis, J. M. Perez-Mato, E. S. Tasci, G. de la Flor and M. I. Aroyo	JAC	August 2014	10	10	1	4805	fe		lead zirconate titanate; symmetry-mode analysis; structural correlations; multiple phases	
Crystal forms in pharmaceutical applications: olanzapine, a gift to crystal chemistry that keeps on giving	S. M. Reutzel-Edens and R. M. Bhardwaj	IUCrJ	November 2020	10	10	8	6178	tr	Open	olanzapine; polymorphs; hydrates; crystal forms; pharmaceuticals; crystallization	4.0 (4)
What macromolecular crystallogenesis tells us - what is needed in the future	R. Giegé	IUCrJ	July 2017	9	10	7	9279	fe	Open	crystal engineering; crystallization predictors; crystallogenesis; crystallizability; crowding; determinant and antideterminant; evolution; packing; self-assembly rules; supramolecularity; surface patches; symmetry and asymmetry	1.5 (2,1)
Discerning best practices in XFEL-based biological crystallography - standards for nonstandard experiments	A. Gorel, I. Schlichting and T. R. M. Barends	IUCrJ	July 2021	9	0	13	3622	fe	Open	serial femtosecond crystallography; data analysis; X-ray free-electron lasers; error models; time-resolved crystallography; extrapolated structure-factor amplitudes; structural biology	2.5 (4,1)
Application of Patterson-function direct methods to materials characterization	J. Rius	IUCrJ	September 2014	9	8	1	8935	fe	Open	direct methods; PFDM; δ recycling; S-FFT; S-TF; cluster-based DM; powder diffraction; ab initio structure solution; precession electron diffraction; electron diffraction tomography	3.0 (3)
MicroED: conception, practice and future opportunities	M. T. B. Clabbers, A. Shiriaeva and T. Gonen	IUCrJ	March 2022	9	6	15	8133	tr	Open	MicroED; cryo-EM; microcrystal electron diffraction; crystallography;	2.5 (4,1)

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										membrane proteins	
Structural biology in the time of COVID-19: perspectives on methods and milestones	M. L. Lynch, E. H. Snell and S. E. J. Bowman	IUCrJ	May 2021	9	9	42	11003	tr	Open	structural biology; SARS-CoV-2; X-ray crystallography; cryoelectron microscopy; COVID-19	3.5 (5,2)
X-ray constrained wavefunctions based on Hirshfeld atoms. I. Method and review	M. L. Davidson, S. Grabowsky and D. Jayatilaka	B	June 2022	9	9	1	2465	tr		X-ray constrained wavefunction; Hirshfeld atom; halting problem; X-ray wavefunction refinement	
Synchrotron radiation micro-tomography for high-resolution neurovascular network morphology investigation	Y. Cao, M. Zhang, H. Ding, Z. Chen, B. Tang, T. Wu, B. Xiao, C. Duan, S. Ni, L. Jiang, Z. Luo, C. Li, J. Zhao, S. Liao, X. Yin, Y. Fu, T. Xiao, H. Lu and J. Hu	JSR	May 2019	8	8	1	1854	tr		high-resolution; imaging; neurovascular network; 3D	4.0 (4)
Stochastic polarity formation in molecular crystals, composite materials and natural tissues	J. Hulliger, M. Burgener, R. Hesterberg, M. Sommer, K. Brahimi and H. Aboulfadl	IUCrJ	July 2017	8	7	3	3995	tr	Open	stochastic polarity formation; molecular crystals; biomimetic materials; natural tissues; Markov chain processes	4.0 (4,4)
Why is interoperability between the two fields of chemical crystallography and protein crystallography so difficult?	A. Brink and J. R. Helliwell	IUCrJ	September 2019	8	8	17	4003	tr	Open	interoperability; chemical crystallography; macromolecular crystallography; Cambridge Structural Database; Protein Data Bank	4.0 (4,4)
Structural biology of coronavirus ion channels	F. J. Barrantes	D	April 2021	7	7	9	3681	tr		coronaviruses; COVID-19; SARS-CoV-2; cryo-electron microscopy; viroporins; structure-function correlations; viral ion channels	3.0 (4,2)
The quaternion-based spatial-coordinate and orientation-frame alignment problems	A. J. Hanson	A	July 2020	7	7	5	3957	la	Open	data alignment; spatial-coordinate alignment; orientation-frame alignment; quaternions; quaternion frames; quaternion eigenvalue methods	3.5 (4,3)
Scanning transmission electron diffraction methods	A. S. Eggeman	B	August 2019	7	9		1743	tr		transmission electron microscopy; scanning	4.0 (4)

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										electron diffraction; precession electron diffraction; electron crystallography	
Ion permeation in potassium ion channels	L. Coates	D	April 2020	7	8	2	3023	tr	Open	ion channels; membrane proteins; X-ray crystallography; anomalous scattering	3.5 (4,3)
HUG and SQUEEZE: using CRYSTALS to incorporate resonant scattering in the SQUEEZE structure-factor contributions to determine absolute structure	R. I. Cooper, H. D. Flack and D. J. Watkin	C	November 2017	7	6	8	2859	fe		disorder; resonsant scattering; absolute structure	4.0 (5,3)
Short X-ray pulses from third-generation light sources	A. G. Stepanov and C. P. Hauri	JSR	January 2016	7	8	1	2626	la	Free	laser slicing; femtosecond X-ray pulses; picosecond X-ray pulses; X-ray pulse compression; X-ray switch	2.0 (3,1)
Bone hierarchical structure: spatial variation across length scales	N. K. Wittig and H. Birkedal	B	June 2022	7	7	2	2657	tr		bone; biomineralization; hierarchical material; X-ray imaging	4.0 (4,4)
The early history of cryo-cooling for macromolecular crystallography	D. J. Haas	IUCrJ	March 2020	6	6	9	5710	tr	Open	cryo-crystallography; cryo-protectant; flash-cooling; X-ray radiation damage; macromolecular crystallography	3.0 (3)
Distortions, deviations and alternative facts: reliability in crystallography	W. Clegg	IUCrJ	January 2021	6	5	36	7897	fe	Open	structural distortions; structure interpretation; structure validation; scientific fraud	5.0 (5)
Cascading time evolution of dissipative structures leading to unique crystalline textures	T. Hashimoto and H. Murase	IUCrJ	January 2015	6	6	1	5638	fe	Open	dissipative structures; shish-kebab structures; extended-chain crystal textures; polymer crystallization	3.0 (3)
X-ray magnetic diffraction under high pressure	Y. Wang, T. F. Rosenbaum and Y. Feng	IUCrJ	July 2019	5	5	1	4564	fe	Open	X-ray magnetic diffraction; resonant X-ray orbital scattering; non-resonant X-ray diffraction of charge orders; high pressure;	3.5 (4,3)

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										cryogenic temperatures; spin-density-wave materials; antiferromagnets	
The crystal structures of the enzyme hydroxymethylbilane synthase, also known as porphobilinogen deaminase	J. R. Helliwell	F	November 2021	5	5	2	1634	tr	Open	hydroxymethylbilane synthase; porphobilinogen deaminase; enzyme-substrate intermediates; reaction mechanisms; structure and function	4.0 (4,4)
Real space in cryo-EM: the future is local	C. M. Palmer and C. H. S. Aylett	D	February 2022	4	3	4	4537	tr	Open	denoising; local resolution; local filtering; noise suppression; real-space measures; real-space filtering; cryo-EM	3.0 (3,3)
Growing a thriving international community for small-angle scattering through collaboration	J. Trewhella	JAC	August 2021	4	3	1	1552	fe	Open	small-angle scattering; SAS; triennial SAS conferences; International Union of Crystallography; IUCr; Guinier Prize; standards	
Epoxide hydrolysis as a model system for understanding flux through a branched reaction scheme	Å. Janfalk Carlsson, P. Bauer, D. Dobritzsch, S. C. L. Kamerlin and M. Widersten	IUCrJ	May 2018	4	5	4	5157	fe	Open	epoxide hydrolase; stereoselectivity; empirical valence-bond simulations; biocatalysis; reaction flux; trans-methylstyrene oxide	3.0 (4,2)
Inflation versus projection sets in aperiodic systems: the role of the window in averaging and diffraction	M. Baake and U. Grimm	A	September 2020	3	3	7	2432	tr	Open	quasicrystals; projection method; inflation rules; diffraction; hyperuniformity	3.5 (4,3)
X-ray techniques for innovation in industry	K. Lawniczak-Jablonska and J. Cutler	IUCrJ	November 2014	3	4	1	5997	fe	Open	X-ray techniques; industry; innovation	4.0 (4,4)
Isotopy classes for 3-periodic net embeddings	S. C. Power, I. A. Baburin and D. M. Proserpio	A	May 2020	3	4	3	3048	la	Open	periodic nets; embedded nets; coordination polymers; isotopy types; crystallographic frameworks	4.5 (5,4)
The future of biomolecular simulation in the pharmaceutical industry: what	T. Edwards, N. Foloppe, S. A. Harris and G. Wells	D	November 2021	3	4	2	2212	tr	Open	biomolecular simulation; molecular docking; in silico drug design;	3.5 (4,3)

Article title	Author(s)	Journal	Issue	Citations (WoS)	Scopus	Altmetric	Views	Category	Access	Keywords	Review scores
we can learn from aerodynamics modelling and weather prediction. Part 1. understanding the physical and computational complexity of in silico drug design										pharmaceutical industry	
Introduction to molecular replacement: a time perspective	E. Dodson	D	July 2021	3	4	7	2958	tr	Open	crystallographic theory; molecular replacement; test cases; history; scoring functions; crystallographic equations; crystal phasing	
6-Phosphogluconate dehydrogenase and its crystal structures	S. Hanau and J. R. Helliwell	F	March 2022	3	2	2	4252	tr	Open	6-phosphogluconate dehydrogenase; homotropic cooperativity; induced fit; allostery; structure and function; drug targets; bionanotechnology	
Remarks on X-ray constrained/restrained wavefunction fitting	H.-B. Bürgi and A. Genoni	B	June 2022	2	3	1	2090	la		Experimental wavefunction; X-ray constrained wavefunction; X-ray restrained wavefunction	
20 years of crystal hits: progress and promise in ultrahigh-throughput crystallization screening	M. L. Lynch, M. E. Snell, S. A. Potter, E. H. Snell, S. E. J. Bowman and C. S. Bond	D	March 2023	1	0	8	1845	fe	Open	macromolecular crystallization; macromolecular crystallography; crystallization facilities; high-throughput crystallization; crystallization screening	2.0 (3,1)
Machine learning for scattering data: strategies, perspectives and applications to surface scattering	A. Hinderhofer, A. Greco, V. Starostin, V. Munteanu, L. Pithan, A. Gerlach, F. Schreiber and J. Hajdu	JAC	February 2023	1	1	1	1530	tr	Open	surface scattering; X-ray diffraction; neutron scattering; machine learning; data analysis	3.0 (4,2)
Using crystallography tools to improve vaccine formulations	M. C. A. Fantini, C. L. P. Oliveira, J. L. S. Lopes, T. S. Martins, M. A. Akamatsu, A. G. Trezena, M. T.-D.- Franco, V. F. Botosso, O. A. B. E. Sant'Anna, N. Kardjilov, M. K. Rasmussen and H. N. Bordallo	IUCrJ	January 2022	1	1	4	2882	tr	Open	oral vaccines; porous silica; SAXS; XAS; imaging	3.0 (3)
CSD Communications of the	G. M. Ferrence, C. A. Tovee, S. J. W. Holgate, N.	IUCrJ	January	1	1	7	2895	tr	Open	Cambridge Structural	4.5

Article title	Author(s)	Journal	Issue	Citations (WoS)	Scopus	Altmetric	Views	Category	Access	Keywords	Review scores
Cambridge Structural Database	T. Johnson, M. P. Lightfoot, K. L. Nowakowska-Orzechowska, S. C. Ward and P. Lightfoot		2023							Database; CSD Communications; data preservation	(5,4)
Understanding structural distortions in hybrid layered perovskites with the n = 1 Ruddlesden-Popper structure	T. Liu, N. P. Holzapfel, P. M. Woodward and P. Lightfoot	IUCrJ	July 2023	1	1	16	1845	fe	Open	perovskites; symmetry mode analysis; organic-inorganic hybrid materials; Ruddlesden-Popper structure	4.7 (5,5,4)
Trends in coordination of rhenium organometallic complexes in the Protein Data Bank	A. Brink, F. J. F. Jacobs and J. R. Helliwell	IUCrJ	March 2022	1	0	3	4395	tr	Open	organometallic complexes; proteins; rhenium; technetium; radiopharmaceuticals; radioisotopes; transition metals	3.7 (4,4,3)
Pathological crystal structures	K. N. Raymond and G. S. Girolami	C	September 2023	1	1		2124	tr	Open	crystallographic errors; atom misassignments; incorrect modeling; disordered guest molecules; incorrect space group; incorrect cell size; checkCIF	5.0 (5,5)
Native glycosylation and binding of the antidepressant paroxetine in a low-resolution crystal structure of human myeloperoxidase	L. Krawczyk, S. Semwal, J. Soubhye, S. Lemri Ouadriri, M. Prévost, P. Van Antwerpen, G. Roos and J. Bouckaert	D	September 2022	1	2	4	2001	fe	Open	human myeloperoxidase; glycosylation; N-glycan refinement; thiocyanate; paroxetine	2.5 (3,2)
On the centennials of the discoveries of the hydrogen bond and the structure of the water molecule: the short life and work of Eustace Jean Cuy (1897-1925)	Z. S. Derewenda	A	September 2021	0	2	4	729	fe		hydrogen bond; water molecule structure; history of structural chemistry	2.0 (3,1)
Deep learning applications in protein crystallography	S. Matinyan, P. Filipcik, J. P. Abrahams and A. Altomare	A	January 2024	0	0		1068	la	Open	protein crystallography; deep learning; artificial intelligence; machine learning	3.5 (4,3)
Facing the phase problem	W. A. Hendrickson and E. N. Baker	IUCrJ	September 2023	0	1		1734	la	Open	anomalous diffraction; density modification; direct methods; isomorphous replacement; molecular replacement	4.0 (4,4)

Article title	Author(s)	Journal	Issue	Citations (WoS)	Scopus	Altmetric	Views	Category	Access	Keywords	Review scores
Going around the Kok cycle of the water oxidation reaction with femtosecond X-ray crystallography	A. Bhowmick, P. S. Simon, I. Bogacz, R. Hussein, M. Zhang, H. Makita, M. Ibrahim, R. Chatterjee, M. D. Doyle, M. H. Cheah, P. Chernev, F. D. Fuller, T. Fransson, R. Alonso-Mori, A. S. Brewster, N. K. Sauter, U. Bergmann, H. Dobbek, A. Zouni, J. Messinger, J. Kern, V. K. Yachandra, J. Yano and T. Ishikawa	IUCrJ	November 2023	0	0		1883	tr	Open	photosystem II; oxygen evolving complex; manganese metalloenzymes; water-oxidation; water-splitting; X-ray free-electron lasers; X-ray spectroscopy	3.5 (4,3)
Structure and function relationship of formate dehydrogenases: an overview of recent progress	A. Kobayashi, M. Taketa, K. Sowa, K. Kano, Y. Higuchi, H. Ogata and J. L. Smith	IUCrJ	September 2023	0	0		569	tr	Open	formate dehydrogenases; biotechnological applications; Methylorubrum extorquens AM1; Mo/W enzymes	4.0 (4)
The interoperability of crystallographic data and databases	A. Brink, I. Bruno, J. Helliwell, B. McMahon and P. Lightfoot	IUCrJ	January 2024	0	0		1448	fe	Open	interoperability; data; databases; interdisciplinarity; cross-domain integration; CODATA	3.5 (4,3)
The African Light Source: history, context and future	S. H. Connell, K. Dollman, G. Kamel, S. A. Khan, E. Mitchell, S. K. Mtingwa, M. C. Newton, P. Ngabonziza, E. Nji, L. Norris, M. Zema and K. Kvashnina	JSR	January 2024	0	0		948	fe	Open	African Light Source; AfLS; synchrotron; history	5.0 (5)
Emergence of liquid following laser melting of gold thin films	I. K. Robinson, J. P. Griffiths, R. Koch, T. A. Assefa, A. F. Suzana, Y. Cao, S. Kim, D. Kim, H. Lee, S. Kim, J. H. Lee, S.-Y. Park, I. Eom, J. Park, D. Nam, S. Kim, S. H. Chun, H. Hyun, K.-S. Kim, M. Lu, C. Song, H. Kim, S. J. L. Billinge, E. S. Bozin and V. K. Peterson	IUCrJ	November 2023	0	0		943	tr	Open	ultrafast X-ray diffraction; laser melting; pair distribution functions; inhomogeneous melting; liquid structure factors	2.5 (3,2)
Correcting systematic errors in diffraction data with modern scaling algorithms	L. A. Aldama, K. M. Dalton, D. R. Hekstra and D. G. Waterman	D	September 2023	0	0		603	tr	Open	X-ray crystallography; scaling; variational inference; deep learning	4.0 (5,3)
From femtoseconds to minutes: time-resolved macromolecular crystallography at XFELs and synchrotrons	N. Caramello, A. Royant and C. Mueller-Dieckmann	D	February 2024	0	0		482	fe	Open	time-resolved serial crystallography; synchrotrons; XFELs; structural photobiology; reaction-intermediate states; bacteriorhodopsin; cryo-trapping	3.7 (4,4,3)
Advice on describing Bayesian analysis of neutron and X-ray reflectometry	A. R. McCluskey, A. J. Caruana, C. J. Kinane, A. J. Armstrong, T. Arnold, J. F. K. Cooper, D. L. Cortie, A. V. Hughes, J.-F. Moulin, A. R. J. Nelson, W. Potrzebowski, V. Starostin and A.	JAC	February 2023	0	0	5	997	fe	Open	reflectometry; reflectivity; Bayesian analysis; FAIR data standards	4.7 (5,5,4)

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	Barty										