



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 05:18 PM JST

PDB ID : 5GJA
Title : Crystal structure of Arabidopsis thaliana ACO2 in complex with 2-PA
Authors : Sun, X.Z.; Li, Y.X.; He, W.R.; Ji, C.G.; Xia, P.X.; Wang, Y.C.; Du, S.; Li, H.J.; Raikhel, N.; Xiao, J.Y.; Guo, H.W.
Deposited on : 2016-06-28
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

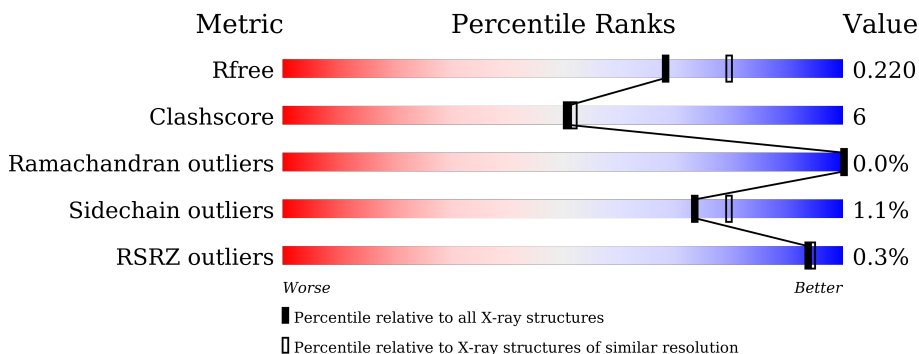
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	90% (green), 9% (yellow), 1% (orange), 0% (red), 0% (grey)
1	B	303	85% (green), 13% (yellow), 2% (orange), 0% (red), 0% (grey)
1	C	303	83% (green), 15% (yellow), 2% (orange), 0% (red), 0% (grey)
1	D	303	87% (green), 10% (yellow), 3% (orange), 0% (red), 0% (grey)
1	E	303	78% (green), 15% (yellow), 5% (orange), 0% (red), 2% (grey)
1	F	303	89% (green), 9% (yellow), 2% (orange), 0% (red), 0% (grey)

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Mol	Chain	Length	Quality of chain
1	G	303	 90% 8%
1	H	303	 79% 16% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20234 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1-aminocyclopropane-1-carboxylate oxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2386	1514	395	463	14	0	0	0
1	B	298	2378	1509	394	462	13	0	0	0
1	C	298	2378	1509	394	462	13	0	0	0
1	D	299	2386	1514	395	463	14	0	0	0
1	E	288	2302	1461	381	448	12	0	0	0
1	F	298	2378	1509	394	462	13	0	0	0
1	G	298	2378	1509	394	462	13	0	0	0
1	H	287	2294	1457	380	445	12	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

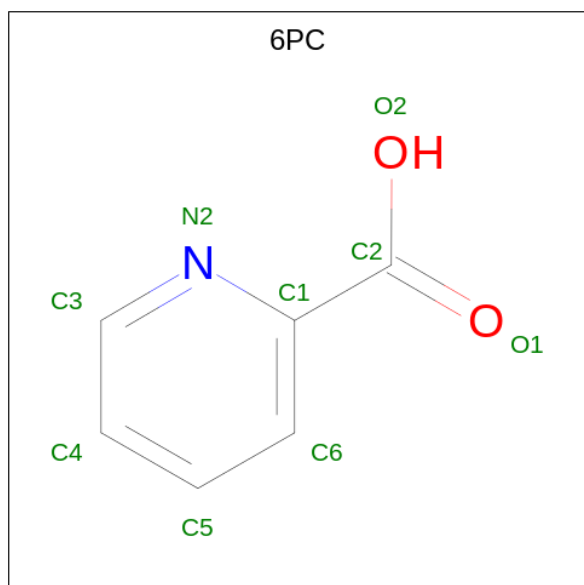
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PYRIDINE-2-CARBOXYLIC ACID (three-letter code: 6PC) (formula: $C_6H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		
3	E	1	Total	C	N	O	0	0
			9	6	1	2		
3	F	1	Total	C	N	O	0	0
			9	6	1	2		
3	G	1	Total	C	N	O	0	0
			9	6	1	2		
3	H	1	Total	C	N	O	0	0
			9	6	1	2		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	178	Total O 178 178	0	0
4	B	156	Total O 156 156	0	0
4	C	149	Total O 149 149	0	0
4	D	183	Total O 183 183	0	0
4	E	130	Total O 130 130	0	0
4	F	178	Total O 178 178	0	0
4	G	159	Total O 159 159	0	0
4	H	141	Total O 141 141	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

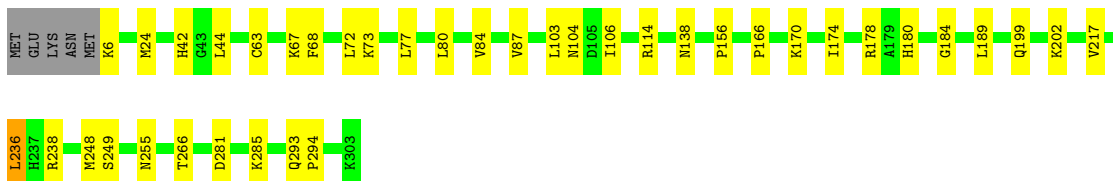
- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain A:  90% 9% .




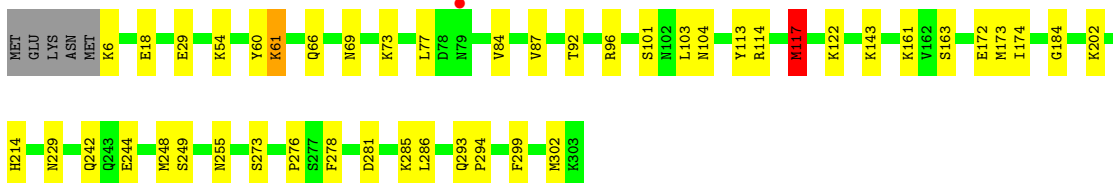
- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain B:  85% 13% .



- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain C:  83% 15% .




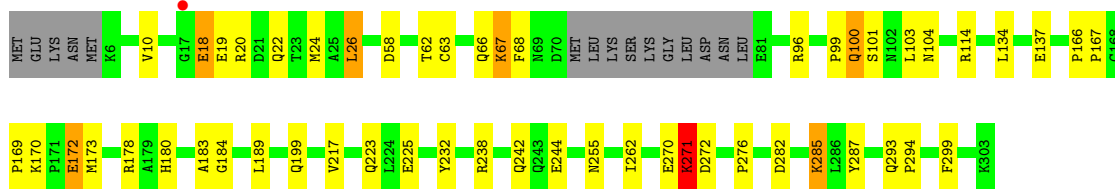
- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain D:  87% 10% ..




- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain E:  78% 15% 5%




- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain F:  89% 9% 2%




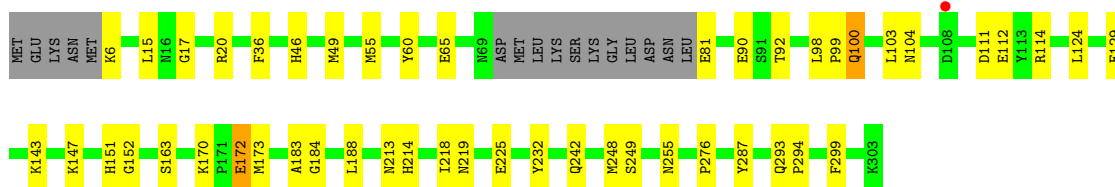
- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain G:  90% 8% 2%



- Molecule 1: 1-aminocyclopropane-1-carboxylate oxidase 2

Chain H:  79% 16% 5%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 95.34Å 95.89Å 90.06° 89.48° 89.99°	Depositor
Resolution (Å)	48.59 – 2.10 48.59 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.59-2.10) 92.0 (48.59-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.171 , 0.218 0.171 , 0.220	Depositor DCC
R_{free} test set	2027 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtrriage
Anisotropy	1.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for h,l,-k 0.000 for h,-l,k 0.055 for h,-k,-l 0.457 for -h,k,-l 0.054 for -h,-k,l 0.000 for -h,l,k 0.000 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20234	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9678e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 6PC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2438	0.60	0/3292
1	B	0.41	0/2430	0.60	1/3282 (0.0%)
1	C	0.41	0/2430	0.64	2/3282 (0.1%)
1	D	0.46	2/2438 (0.1%)	0.67	4/3292 (0.1%)
1	E	0.45	2/2353 (0.1%)	0.66	1/3179 (0.0%)
1	F	0.44	1/2430 (0.0%)	0.66	2/3282 (0.1%)
1	G	0.39	0/2430	0.63	2/3282 (0.1%)
1	H	0.39	0/2345	0.66	1/3168 (0.0%)
All	All	0.42	5/19294 (0.0%)	0.64	13/26059 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	GLU	CD-OE1	-7.35	1.17	1.25
1	D	18	GLU	CD-OE1	-7.23	1.17	1.25
1	F	112	GLU	CD-OE1	-5.86	1.19	1.25
1	E	18	GLU	CD-OE2	-5.84	1.19	1.25
1	D	18	GLU	CD-OE2	-5.59	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	55	MET	CG-SD-CE	-11.18	82.31	100.20
1	D	170	LYS	CB-CG-CD	-10.80	83.51	111.60
1	G	154	LYS	CD-CE-NZ	-9.32	90.26	111.70
1	B	236	LEU	CB-CG-CD2	-9.24	95.30	111.00
1	D	170	LYS	CD-CE-NZ	8.27	130.73	111.70
1	C	117	MET	CA-CB-CG	8.17	127.20	113.30
1	H	100	GLN	CA-CB-CG	-7.97	95.88	113.40
1	F	112	GLU	OE1-CD-OE2	7.50	132.29	123.30
1	E	26	LEU	CB-CG-CD2	-6.86	99.33	111.00
1	D	170	LYS	CG-CD-CE	6.57	131.60	111.90
1	D	170	LYS	CA-CB-CG	6.53	127.77	113.40
1	C	117	MET	CB-CG-SD	5.39	128.56	112.40
1	G	16	ASN	N-CA-C	5.25	125.16	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	100	GLN	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	0	2338	18	0
1	B	2378	0	2329	25	1
1	C	2378	0	2329	33	0
1	D	2386	0	2338	26	0
1	E	2302	0	2242	44	0
1	F	2378	0	2329	20	0
1	G	2378	0	2329	12	0
1	H	2294	0	2238	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
3	C	9	0	4	0	0
3	D	9	0	4	0	0
3	E	9	0	4	0	0
3	F	9	0	4	0	0
3	G	9	0	4	0	0
3	H	9	0	4	0	0
4	A	178	0	0	2	0
4	B	156	0	0	2	0
4	C	149	0	0	8	0
4	D	183	0	0	1	0
4	E	130	0	0	4	1
4	F	178	0	0	3	0
4	G	159	0	0	1	0
4	H	141	0	0	4	0
All	All	20234	0	18504	213	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:LYS:HE2	1:H:173:MET:HG3	1.30	1.14
1:H:172:GLU:HG2	1:H:173:MET:HE3	1.57	0.86
1:E:18:GLU:OE2	4:E:501:HOH:O	1.97	0.82
1:H:99:PRO:O	1:H:100:GLN:HG2	1.81	0.80
1:E:20:ARG:NH1	4:E:502:HOH:O	2.13	0.80
1:B:103:LEU:HG	1:B:114:ARG:HG3	1.69	0.73
1:E:67:LYS:H	1:E:67:LYS:HE2	1.52	0.73
1:D:73:LYS:HE3	1:D:78:ASP:HB3	1.70	0.72
1:C:103:LEU:HG	1:C:114:ARG:HG3	1.70	0.72
1:A:199:GLN:HE22	1:A:238:ARG:HH21	1.39	0.70
1:H:213:ASN:HD22	1:H:214:HIS:HD2	1.35	0.70
1:C:18:GLU:HB3	1:H:143:LYS:NZ	2.06	0.70
1:D:170:LYS:HD3	1:D:173:MET:HG3	1.74	0.70
1:B:84:VAL:HG11	1:B:87:VAL:HG22	1.73	0.70
1:D:170:LYS:CD	1:D:173:MET:HG3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:GLN:HE22	1:D:238:ARG:HH21	1.41	0.68
1:E:99:PRO:C	1:E:100:GLN:HG2	2.13	0.68
1:C:281:ASP:O	1:C:285:LYS:HG2	1.94	0.67
1:E:96:ARG:NH2	4:E:503:HOH:O	2.21	0.67
1:C:113:TYR:O	1:C:117:MET:HB2	1.95	0.67
1:G:99:PRO:C	1:G:100:GLN:HG2	2.13	0.67
1:B:199:GLN:HE22	1:B:238:ARG:HH21	1.43	0.67
1:F:213:ASN:HD22	1:F:214:HIS:CD2	2.13	0.66
1:H:213:ASN:HD22	1:H:214:HIS:CD2	2.12	0.66
1:C:77:LEU:HD11	1:C:87:VAL:HG21	1.78	0.65
1:A:47:ASP:O	1:A:51:LYS:HG2	1.97	0.65
1:E:66:GLN:N	1:E:66:GLN:OE1	2.27	0.65
1:D:80:LEU:O	1:D:170:LYS:NZ	2.24	0.65
1:E:24:MET:HE3	1:E:134:LEU:HD22	1.78	0.64
1:E:199:GLN:HE22	1:E:238:ARG:HH21	1.46	0.63
1:A:103:LEU:HG	1:A:114:ARG:HG3	1.80	0.63
1:B:84:VAL:CG1	1:B:87:VAL:HG22	2.29	0.63
1:F:51:LYS:O	1:F:55:MET:HG3	1.99	0.63
1:F:55:MET:HE1	1:F:112:GLU:OE1	1.98	0.63
1:H:20:ARG:NH2	4:H:503:HOH:O	2.30	0.63
1:E:104:ASN:OD1	1:E:114:ARG:HD3	1.99	0.62
1:D:103:LEU:HG	1:D:114:ARG:HG3	1.81	0.61
1:C:84:VAL:HG11	1:C:87:VAL:HG22	1.82	0.61
1:E:282:ASP:O	1:E:285:LYS:HE3	2.00	0.61
1:G:172:GLU:HG2	1:G:173:MET:HE3	1.82	0.61
1:E:10:VAL:HG22	1:E:26:LEU:HD23	1.82	0.60
1:D:220:LEU:HD12	1:D:224:LEU:HD12	1.84	0.60
1:H:103:LEU:HG	1:H:114:ARG:HG3	1.83	0.60
1:D:170:LYS:HE2	1:D:173:MET:HG3	1.84	0.60
1:A:172:GLU:HG2	1:A:173:MET:HE3	1.84	0.59
1:C:84:VAL:CG1	1:C:87:VAL:HG22	2.33	0.59
1:G:97:HIS:HE1	1:G:160:THR:OG1	1.86	0.58
1:H:20:ARG:NH1	4:H:505:HOH:O	2.36	0.58
1:E:99:PRO:O	1:E:100:GLN:HG2	2.03	0.58
1:F:231:LYS:NZ	4:F:502:HOH:O	2.33	0.58
1:C:202:LYS:NZ	4:C:504:HOH:O	2.37	0.58
1:H:81:GLU:OE1	1:H:170:LYS:NZ	2.27	0.58
1:E:270:GLU:O	1:E:271:LYS:HB2	2.03	0.57
1:B:63:CYS:O	1:B:67:LYS:NZ	2.37	0.57
1:E:169:PRO:HB2	1:E:170:LYS:HD3	1.84	0.57
1:C:66:GLN:NE2	4:C:501:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASP:OD2	4:D:501:HOH:O	2.17	0.56
1:D:170:LYS:HD3	1:D:173:MET:CG	2.36	0.56
1:E:19:GLU:HA	1:E:22:GLN:HE22	1.70	0.56
1:A:148:LYS:NZ	4:A:504:HOH:O	2.37	0.56
1:F:69:ASN:HA	1:F:72:LEU:CD1	2.36	0.56
1:C:69:ASN:HB2	4:C:503:HOH:O	2.06	0.56
1:D:220:LEU:HD12	1:D:224:LEU:CD1	2.36	0.56
1:B:178:ARG:O	1:B:180:HIS:HD2	1.90	0.55
1:D:248:MET:HG2	1:D:249:SER:N	2.22	0.54
1:E:242:GLN:NE2	4:E:504:HOH:O	2.25	0.54
1:D:69:ASN:O	1:D:73:LYS:HD2	2.07	0.54
1:B:281:ASP:O	1:B:285:LYS:HG2	2.08	0.54
1:H:242:GLN:NE2	4:H:507:HOH:O	2.40	0.53
1:B:236:LEU:HD21	1:D:297:PRO:HG3	1.91	0.53
1:H:99:PRO:C	1:H:100:GLN:HG2	2.26	0.53
1:B:77:LEU:HD11	1:B:87:VAL:HG21	1.91	0.53
1:E:63:CYS:O	1:E:67:LYS:HE3	2.09	0.53
1:H:65:GLU:N	4:H:504:HOH:O	2.32	0.53
1:C:18:GLU:HB3	1:H:143:LYS:HZ3	1.73	0.53
1:E:178:ARG:O	1:E:180:HIS:HD2	1.91	0.53
1:A:248:MET:HG2	1:A:249:SER:N	2.24	0.52
1:B:202:LYS:NZ	4:B:509:HOH:O	2.42	0.52
1:E:271:LYS:HG3	1:E:272:ASP:H	1.75	0.52
1:B:199:GLN:HE21	1:B:238:ARG:HE	1.57	0.52
1:C:6:LYS:N	4:C:506:HOH:O	2.42	0.52
1:F:69:ASN:HA	1:F:72:LEU:HD12	1.92	0.52
1:G:161:LYS:HE2	1:G:163:SER:OG	2.10	0.52
1:C:122:LYS:NZ	4:C:505:HOH:O	2.37	0.52
1:A:68:PHE:CE2	1:A:166:PRO:HG2	2.45	0.51
1:A:79:ASN:ND2	1:A:81:GLU:HG3	2.25	0.51
1:E:103:LEU:HG	1:E:114:ARG:HG3	1.92	0.51
1:A:9:VAL:O	4:A:501:HOH:O	2.19	0.51
1:E:167:PRO:HB3	1:E:244:GLU:HA	1.93	0.51
1:E:68:PHE:CE2	1:E:166:PRO:HG2	2.46	0.51
1:F:68:PHE:O	1:F:72:LEU:HD12	2.09	0.51
1:C:242:GLN:NE2	1:C:244:GLU:O	2.35	0.51
1:B:42:HIS:ND1	1:B:44:LEU:HD12	2.26	0.50
1:D:199:GLN:NE2	1:D:238:ARG:HE	2.10	0.50
1:A:199:GLN:NE2	1:A:238:ARG:HE	2.09	0.50
1:E:199:GLN:NE2	1:E:238:ARG:HE	2.10	0.50
1:D:184:GLY:HA3	1:D:255:ASN:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:GLU:HG2	1:E:173:MET:HE3	1.94	0.50
1:B:199:GLN:NE2	1:B:238:ARG:HE	2.11	0.49
1:F:213:ASN:HD22	1:F:214:HIS:HD2	1.56	0.49
1:B:104:ASN:OD1	1:B:114:ARG:HD2	2.12	0.49
1:C:18:GLU:HB3	1:H:143:LYS:HZ1	1.74	0.49
1:D:68:PHE:CE2	1:D:166:PRO:HG2	2.48	0.49
1:E:199:GLN:HE21	1:E:238:ARG:HE	1.60	0.49
1:A:199:GLN:HE21	1:A:238:ARG:HE	1.59	0.49
1:H:170:LYS:HG3	1:H:173:MET:HB2	1.95	0.49
1:B:106:ILE:O	4:B:501:HOH:O	2.20	0.49
1:C:172:GLU:HB2	1:C:173:MET:HE3	1.95	0.48
1:D:74:SER:O	1:G:79:ASN:HB3	2.13	0.48
1:C:61:LYS:O	4:C:501:HOH:O	2.20	0.48
1:E:67:LYS:HE2	1:E:67:LYS:N	2.26	0.48
1:F:90:GLU:HG2	1:F:92:THR:HG23	1.95	0.48
1:H:184:GLY:HA3	1:H:255:ASN:ND2	2.28	0.47
1:A:184:GLY:HA3	1:A:255:ASN:OD1	2.15	0.47
1:B:68:PHE:CE2	1:B:166:PRO:HG2	2.50	0.47
1:C:229:ASN:ND2	1:C:273:SER:OG	2.48	0.47
1:E:170:LYS:HB3	1:E:172:GLU:OE2	2.15	0.47
1:H:46:HIS:HA	1:H:49:MET:HE3	1.97	0.47
1:G:95:VAL:HG22	1:G:106:ILE:CD1	2.45	0.46
1:H:225:GLU:HA	1:H:232:TYR:O	2.15	0.46
1:D:170:LYS:CE	1:D:173:MET:HG3	2.45	0.46
1:G:235:VAL:O	1:G:237:HIS:HD2	1.96	0.46
1:H:188:LEU:HD22	1:H:218:ILE:HD12	1.96	0.46
1:H:183:ALA:HB2	1:H:287:TYR:CD1	2.51	0.46
1:D:235:VAL:O	1:D:237:HIS:HD2	1.98	0.46
1:H:163:SER:HB2	1:H:249:SER:HB3	1.98	0.46
1:B:80:LEU:O	1:B:170:LYS:HE2	2.16	0.46
1:E:276:PRO:HG3	1:E:299:PHE:O	2.16	0.46
1:C:87:VAL:HG23	1:C:174:ILE:HD11	1.97	0.45
1:E:282:ASP:O	1:E:285:LYS:HG3	2.16	0.45
1:E:20:ARG:NH2	1:E:137:GLU:OE1	2.50	0.45
1:F:63:CYS:SG	1:F:108:ASP:HB2	2.56	0.45
1:C:161:LYS:NZ	4:C:508:HOH:O	2.48	0.45
1:E:66:GLN:HG2	1:E:67:LYS:HZ3	1.81	0.45
1:C:172:GLU:CD	1:C:172:GLU:H	2.20	0.45
1:F:163:SER:HB2	1:F:249:SER:HB3	1.99	0.45
1:E:293:GLN:HB3	1:E:294:PRO:HD2	1.98	0.45
1:H:55:MET:SD	1:H:112:GLU:HG3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLU:OE1	1:H:17:GLY:HA2	2.16	0.45
1:A:70:ASP:O	1:A:73:LYS:HE3	2.17	0.45
1:C:92:THR:HG22	1:C:163:SER:OG	2.17	0.44
1:C:104:ASN:OD1	1:C:114:ARG:HD2	2.17	0.44
1:E:223:GLN:NE2	1:E:262:ILE:HG21	2.32	0.44
1:A:244:GLU:CD	1:A:245:GLY:H	2.20	0.44
1:C:66:GLN:H	1:C:66:GLN:CD	2.20	0.44
1:E:225:GLU:HA	1:E:232:TYR:O	2.18	0.44
1:H:293:GLN:HB3	1:H:294:PRO:HD2	1.99	0.44
1:C:60:TYR:HD2	1:C:61:LYS:HZ2	1.63	0.44
1:E:19:GLU:HA	1:E:22:GLN:NE2	2.32	0.44
1:G:242:GLN:NE2	1:G:244:GLU:O	2.50	0.44
1:F:183:ALA:HB2	1:F:287:TYR:CD2	2.53	0.44
1:B:24:MET:HB3	1:B:138:ASN:HD21	1.82	0.44
1:H:276:PRO:HG3	1:H:299:PHE:O	2.17	0.44
1:F:172:GLU:HG2	1:F:173:MET:HE3	1.99	0.44
1:C:184:GLY:HA3	1:C:255:ASN:OD1	2.17	0.44
1:B:87:VAL:HG23	1:B:174:ILE:HD11	2.00	0.43
1:E:184:GLY:HA3	1:E:255:ASN:ND2	2.33	0.43
1:F:55:MET:HE2	1:F:113:TYR:HB2	2.00	0.43
1:A:266:THR:HG22	4:F:601:HOH:O	2.17	0.43
1:D:293:GLN:HB3	1:D:294:PRO:HD2	1.99	0.43
1:E:183:ALA:HB2	1:E:287:TYR:CD1	2.53	0.43
1:G:183:ALA:HB2	1:G:287:TYR:CD1	2.53	0.43
1:H:98:LEU:HA	1:H:99:PRO:C	2.39	0.43
1:H:248:MET:HG2	1:H:249:SER:N	2.33	0.43
1:C:248:MET:HG2	1:C:249:SER:N	2.33	0.43
1:H:46:HIS:CD2	1:H:49:MET:HE3	2.53	0.43
1:B:72:LEU:HD22	1:B:77:LEU:HB2	1.99	0.43
1:C:96:ARG:O	1:C:101:SER:HA	2.18	0.43
1:E:63:CYS:C	1:E:67:LYS:HZ2	2.20	0.43
1:E:271:LYS:HG3	1:E:272:ASP:N	2.34	0.43
1:C:214:HIS:HD2	4:C:639:HOH:O	2.01	0.42
1:G:103:LEU:HG	1:G:114:ARG:HG3	2.02	0.42
1:E:96:ARG:O	1:E:101:SER:HA	2.18	0.42
1:H:15:LEU:O	1:H:20:ARG:HD2	2.19	0.42
1:H:188:LEU:HD22	1:H:218:ILE:CD1	2.48	0.42
1:G:97:HIS:HD2	4:G:647:HOH:O	2.02	0.42
1:E:58:ASP:O	1:E:62:THR:HG23	2.19	0.42
1:H:151:HIS:HD2	1:H:152:GLY:O	2.00	0.42
1:B:248:MET:HG2	1:B:249:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:PRO:HG3	1:C:299:PHE:O	2.19	0.42
1:D:50:ASP:OD1	1:D:214:HIS:HE1	2.03	0.42
1:D:109:VAL:HG23	1:D:113:TYR:CD2	2.54	0.42
1:F:18:GLU:C	1:F:20:ARG:N	2.72	0.42
1:H:81:GLU:OE1	1:H:81:GLU:HA	2.20	0.42
1:H:104:ASN:OD1	1:H:114:ARG:HD2	2.20	0.42
1:B:266:THR:HG21	1:H:111:ASP:OD1	2.20	0.42
1:B:293:GLN:HB3	1:B:294:PRO:HD2	2.02	0.42
1:A:213:ASN:HD21	1:A:214:HIS:CE1	2.38	0.41
1:C:293:GLN:HB3	1:C:294:PRO:HD2	2.02	0.41
1:F:172:GLU:CG	1:F:173:MET:HE3	2.50	0.41
1:F:114:ARG:HD3	4:F:504:HOH:O	2.20	0.41
1:B:184:GLY:HA3	1:B:255:ASN:OD1	2.20	0.41
1:F:184:GLY:HA3	1:F:255:ASN:OD1	2.21	0.41
1:D:14:LYS:HD3	1:D:19:GLU:OE1	2.21	0.41
1:G:36:PHE:CD2	1:G:219:ASN:HB3	2.56	0.41
1:B:189:LEU:HB3	1:B:217:VAL:HB	2.02	0.41
1:F:276:PRO:HG3	1:F:299:PHE:O	2.21	0.41
1:H:36:PHE:CD2	1:H:219:ASN:HB3	2.56	0.41
1:H:60:TYR:CE2	1:H:65:GLU:HB2	2.55	0.41
1:H:90:GLU:HG2	1:H:92:THR:HG23	2.02	0.41
1:H:170:LYS:HE2	1:H:173:MET:CG	2.23	0.41
1:H:124:LEU:HB3	1:H:188:LEU:HD12	2.03	0.41
1:D:199:GLN:HE21	1:D:238:ARG:HE	1.68	0.40
1:E:20:ARG:HH21	1:E:137:GLU:CD	2.25	0.40
1:C:278:PHE:HB2	1:C:302:MET:HE3	2.03	0.40
1:E:189:LEU:HB3	1:E:217:VAL:HB	2.04	0.40
1:H:129:GLU:OE2	1:H:147:LYS:NZ	2.53	0.40
1:E:67:LYS:HE2	1:E:67:LYS:HB2	1.81	0.40
1:F:55:MET:HE2	1:F:55:MET:HB3	1.75	0.40
1:A:79:ASN:HD21	1:A:81:GLU:HG3	1.87	0.40
1:D:42:HIS:ND1	1:D:44:LEU:HD12	2.36	0.40
1:A:172:GLU:HG2	1:A:173:MET:CE	2.51	0.40
1:H:92:THR:HG22	1:H:163:SER:OG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:O	4:E:501:HOH:O[1_545]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/303 (98%)	294 (99%)	3 (1%)	0	100	100
1	B	296/303 (98%)	292 (99%)	4 (1%)	0	100	100
1	C	296/303 (98%)	290 (98%)	6 (2%)	0	100	100
1	D	297/303 (98%)	293 (99%)	4 (1%)	0	100	100
1	E	284/303 (94%)	280 (99%)	3 (1%)	1 (0%)	34	32
1	F	296/303 (98%)	289 (98%)	7 (2%)	0	100	100
1	G	296/303 (98%)	288 (97%)	8 (3%)	0	100	100
1	H	283/303 (93%)	279 (99%)	4 (1%)	0	100	100
All	All	2345/2424 (97%)	2305 (98%)	39 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	271	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/271 (98%)	264 (99%)	3 (1%)	73	79
1	B	266/271 (98%)	264 (99%)	2 (1%)	81	86
1	C	266/271 (98%)	260 (98%)	6 (2%)	50	55
1	D	267/271 (98%)	264 (99%)	3 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	257/271 (95%)	253 (98%)	4 (2%)	62	69
1	F	266/271 (98%)	264 (99%)	2 (1%)	81	86
1	G	266/271 (98%)	264 (99%)	2 (1%)	81	86
1	H	256/271 (94%)	254 (99%)	2 (1%)	81	86
All	All	2111/2168 (97%)	2087 (99%)	24 (1%)	73	79

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	148	LYS
1	A	286	LEU
1	B	73	LYS
1	B	156	PRO
1	C	54	LYS
1	C	61	LYS
1	C	73	LYS
1	C	117	MET
1	C	143	LYS
1	C	286	LEU
1	D	18	GLU
1	D	44	LEU
1	D	73	LYS
1	E	67	LYS
1	E	172	GLU
1	E	271	LYS
1	E	285	LYS
1	F	6	LYS
1	F	286	LEU
1	G	73	LYS
1	G	285	LYS
1	H	6	LYS
1	H	172	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	199	GLN
1	A	213	ASN

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Mol	Chain	Res	Type
1	A	293	GLN
1	B	138	ASN
1	B	180	HIS
1	B	199	GLN
1	B	214	HIS
1	B	293	GLN
1	C	223	GLN
1	C	229	ASN
1	D	46	HIS
1	D	199	GLN
1	D	214	HIS
1	D	237	HIS
1	E	33	ASN
1	E	41	ASN
1	E	180	HIS
1	E	199	GLN
1	E	213	ASN
1	E	214	HIS
1	E	223	GLN
1	E	255	ASN
1	E	293	GLN
1	F	33	ASN
1	F	214	HIS
1	F	229	ASN
1	F	243	GLN
1	F	293	GLN
1	G	97	HIS
1	G	237	HIS
1	H	28	ASN
1	H	33	ASN
1	H	41	ASN
1	H	46	HIS
1	H	214	HIS
1	H	255	ASN
1	H	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PC	C	402	2	9,9,9	1.05	1 (11%)	11,11,11	1.51	2 (18%)
3	6PC	B	402	2	9,9,9	0.79	0	11,11,11	1.86	3 (27%)
3	6PC	D	402	2	9,9,9	0.89	0	11,11,11	1.99	4 (36%)
3	6PC	F	402	2	9,9,9	0.80	0	11,11,11	1.74	4 (36%)
3	6PC	H	402	2	9,9,9	1.00	0	11,11,11	1.45	2 (18%)
3	6PC	E	402	2	9,9,9	0.94	0	11,11,11	1.76	4 (36%)
3	6PC	A	402	2	9,9,9	1.09	1 (11%)	11,11,11	1.53	4 (36%)
3	6PC	G	402	2	9,9,9	0.99	0	11,11,11	1.80	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PC	C	402	2	-	0/4/4/4	0/1/1/1
3	6PC	B	402	2	-	0/4/4/4	0/1/1/1
3	6PC	D	402	2	-	0/4/4/4	0/1/1/1
3	6PC	F	402	2	-	0/4/4/4	0/1/1/1
3	6PC	H	402	2	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PC	E	402	2	-	0/4/4/4	0/1/1/1
3	6PC	A	402	2	-	0/4/4/4	0/1/1/1
3	6PC	G	402	2	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	6PC	O1-C2	2.17	1.29	1.22
3	C	402	6PC	O1-C2	2.01	1.28	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	6PC	C3-N2-C1	3.95	122.06	116.93
3	B	402	6PC	C3-N2-C1	3.62	121.62	116.93
3	G	402	6PC	C4-C3-N2	-3.60	117.54	123.43
3	D	402	6PC	C3-N2-C1	3.34	121.26	116.93
3	C	402	6PC	C3-N2-C1	3.24	121.13	116.93
3	D	402	6PC	O2-C2-C1	3.07	121.67	114.69
3	A	402	6PC	C3-N2-C1	3.02	120.85	116.93
3	H	402	6PC	C4-C3-N2	-3.01	118.51	123.43
3	H	402	6PC	C3-N2-C1	2.96	120.77	116.93
3	E	402	6PC	O2-C2-C1	2.89	121.27	114.69
3	C	402	6PC	C4-C3-N2	-2.89	118.71	123.43
3	B	402	6PC	C4-C3-N2	-2.81	118.84	123.43
3	D	402	6PC	C4-C3-N2	-2.80	118.86	123.43
3	F	402	6PC	O2-C2-C1	2.77	120.98	114.69
3	F	402	6PC	C4-C3-N2	-2.74	118.95	123.43
3	F	402	6PC	C3-N2-C1	2.64	120.36	116.93
3	B	402	6PC	O2-C2-C1	2.61	120.62	114.69
3	F	402	6PC	O1-C2-C1	-2.60	115.96	121.24
3	E	402	6PC	C4-C3-N2	-2.55	119.26	123.43
3	D	402	6PC	O1-C2-C1	-2.54	116.09	121.24
3	E	402	6PC	C3-N2-C1	2.50	120.18	116.93
3	A	402	6PC	C4-C3-N2	-2.32	119.63	123.43
3	E	402	6PC	O1-C2-C1	-2.19	116.81	121.24
3	A	402	6PC	C2-C1-N2	2.14	121.39	117.54
3	A	402	6PC	C6-C1-N2	-2.12	119.83	122.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/303 (98%)	-0.42	1 (0%) 94 94	15, 30, 61, 97	0
1	B	298/303 (98%)	-0.37	0 100 100	20, 35, 66, 105	0
1	C	298/303 (98%)	-0.37	1 (0%) 94 94	20, 35, 67, 102	0
1	D	299/303 (98%)	-0.42	1 (0%) 94 94	17, 31, 62, 100	0
1	E	288/303 (95%)	-0.31	1 (0%) 94 94	20, 37, 75, 101	0
1	F	298/303 (98%)	-0.38	0 100 100	18, 32, 70, 97	0
1	G	298/303 (98%)	-0.36	1 (0%) 94 94	18, 32, 70, 99	0
1	H	287/303 (94%)	-0.30	1 (0%) 94 94	19, 36, 76, 104	0
All	All	2365/2424 (97%)	-0.37	6 (0%) 94 94	15, 34, 69, 105	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	GLY	2.2
1	C	79	ASN	2.1
1	D	5	MET	2.1
1	A	5	MET	2.1
1	H	108	ASP	2.1
1	G	16	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	6PC	A	402	9/9	0.97	0.09	17,21,25,26	0
3	6PC	B	402	9/9	0.97	0.08	18,22,26,27	0
3	6PC	C	402	9/9	0.97	0.09	18,23,27,28	0
3	6PC	D	402	9/9	0.98	0.10	17,22,27,30	0
3	6PC	F	402	9/9	0.98	0.08	17,22,27,29	0
3	6PC	G	402	9/9	0.98	0.09	16,19,25,25	0
3	6PC	H	402	9/9	0.98	0.09	15,19,30,31	0
3	6PC	E	402	9/9	0.99	0.07	21,25,30,31	0
2	ZN	A	401	1/1	1.00	0.07	22,22,22,22	0
2	ZN	B	401	1/1	1.00	0.08	20,20,20,20	0
2	ZN	C	401	1/1	1.00	0.08	21,21,21,21	0
2	ZN	D	401	1/1	1.00	0.08	21,21,21,21	0
2	ZN	E	401	1/1	1.00	0.07	25,25,25,25	0
2	ZN	F	401	1/1	1.00	0.09	23,23,23,23	0
2	ZN	G	401	1/1	1.00	0.08	21,21,21,21	0
2	ZN	H	401	1/1	1.00	0.07	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.