Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 08:04 PM JST

PDB ID	:	4YJL
Title	:	Crystal structure of APC-ARM in complexed with Amer1-A2
Authors	:	Zhang, Z.; Xiao, Y.; Wu, G.
Deposited on	:	2015-03-03
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:

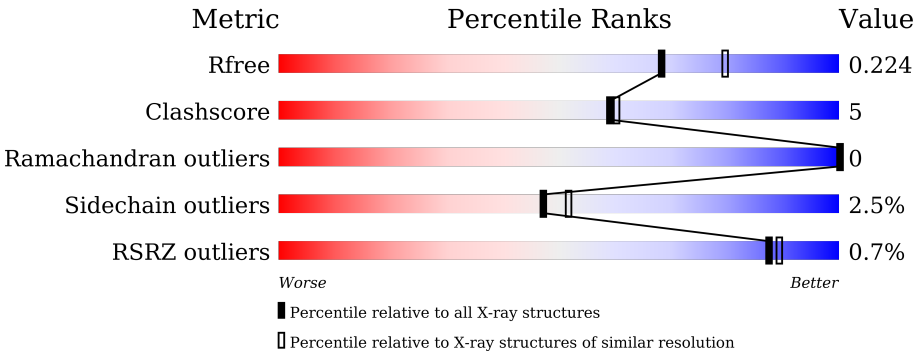
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=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	354	82% 12% • 5%
1	B	354	86% 8% • 5%
1	C	354	86% 8% • 5%
1	D	354	88% 7% • •
1	E	354	87% 8% • •
1	F	354	87% 8% • •

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Mol	Chain	Length	Quality of chain
2	G	13	92% 8%
2	H	13	92% 8%
2	I	13	100%
2	J	13	92% 8%
2	K	13	85% 15%
2	L	13	92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	808	-	-	X	-
3	EDO	D	805	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18962 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 Adenomatous polyposis coli protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2620	1628	478	487	27			
1	B	337	Total	C	N	O	S	0	0	0
			2615	1626	474	488	27			
1	C	338	Total	C	N	O	S	0	0	0
			2625	1632	477	489	27			
1	D	339	Total	C	N	O	S	0	0	0
			2634	1638	479	490	27			
1	E	339	Total	C	N	O	S	0	0	0
			2634	1638	479	490	27			
1	F	339	Total	C	N	O	S	0	0	0
			2634	1638	479	490	27			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	MET	-	expression tag	UNP P25054
A	399	GLY	-	expression tag	UNP P25054
A	400	HIS	-	expression tag	UNP P25054
A	401	HIS	-	expression tag	UNP P25054
A	402	HIS	-	expression tag	UNP P25054
A	403	HIS	-	expression tag	UNP P25054
A	404	HIS	-	expression tag	UNP P25054
A	405	HIS	-	expression tag	UNP P25054
A	406	MET	-	expression tag	UNP P25054
B	398	MET	-	expression tag	UNP P25054
B	399	GLY	-	expression tag	UNP P25054
B	400	HIS	-	expression tag	UNP P25054
B	401	HIS	-	expression tag	UNP P25054
B	402	HIS	-	expression tag	UNP P25054
B	403	HIS	-	expression tag	UNP P25054
B	404	HIS	-	expression tag	UNP P25054
B	405	HIS	-	expression tag	UNP P25054

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Chain	Residue	Modelled	Actual	Comment	Reference
B	406	MET	-	expression tag	UNP P25054
C	398	MET	-	expression tag	UNP P25054
C	399	GLY	-	expression tag	UNP P25054
C	400	HIS	-	expression tag	UNP P25054
C	401	HIS	-	expression tag	UNP P25054
C	402	HIS	-	expression tag	UNP P25054
C	403	HIS	-	expression tag	UNP P25054
C	404	HIS	-	expression tag	UNP P25054
C	405	HIS	-	expression tag	UNP P25054
C	406	MET	-	expression tag	UNP P25054
D	398	MET	-	expression tag	UNP P25054
D	399	GLY	-	expression tag	UNP P25054
D	400	HIS	-	expression tag	UNP P25054
D	401	HIS	-	expression tag	UNP P25054
D	402	HIS	-	expression tag	UNP P25054
D	403	HIS	-	expression tag	UNP P25054
D	404	HIS	-	expression tag	UNP P25054
D	405	HIS	-	expression tag	UNP P25054
D	406	MET	-	expression tag	UNP P25054
E	398	MET	-	expression tag	UNP P25054
E	399	GLY	-	expression tag	UNP P25054
E	400	HIS	-	expression tag	UNP P25054
E	401	HIS	-	expression tag	UNP P25054
E	402	HIS	-	expression tag	UNP P25054
E	403	HIS	-	expression tag	UNP P25054
E	404	HIS	-	expression tag	UNP P25054
E	405	HIS	-	expression tag	UNP P25054
E	406	MET	-	expression tag	UNP P25054
F	398	MET	-	expression tag	UNP P25054
F	399	GLY	-	expression tag	UNP P25054
F	400	HIS	-	expression tag	UNP P25054
F	401	HIS	-	expression tag	UNP P25054
F	402	HIS	-	expression tag	UNP P25054
F	403	HIS	-	expression tag	UNP P25054
F	404	HIS	-	expression tag	UNP P25054
F	405	HIS	-	expression tag	UNP P25054
F	406	MET	-	expression tag	UNP P25054

- Molecule 2 is a protein called APC membrane recruitment protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	13	Total	C	N	O	0	1	0
			115	76	16	23			

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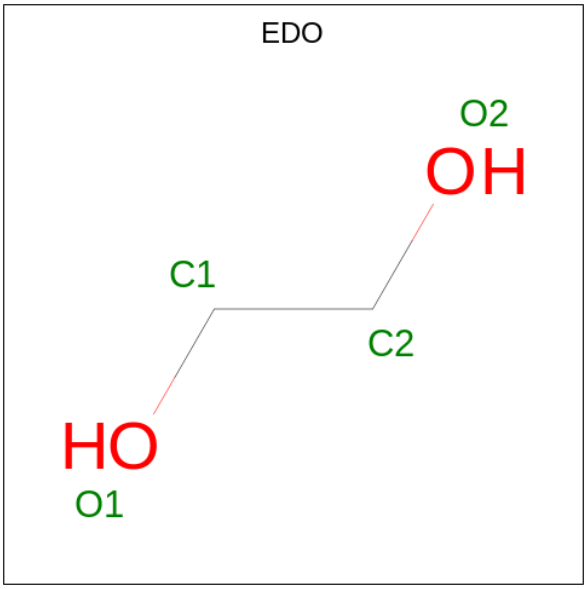
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	13	Total C N O 108 68 16 24	0	0	0
2	I	13	Total C N O 108 68 16 24	0	0	0
2	J	13	Total C N O 108 68 16 24	0	0	0
2	K	13	Total C N O 108 68 16 24	0	0	0
2	L	13	Total C N O 108 68 16 24	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	378	Total O 378 378	0	0
4	B	347	Total O 347 347	0	0
4	C	367	Total O 367 367	0	0
4	D	381	Total O 381 381	0	0
4	E	367	Total O 367 367	0	0
4	F	381	Total O 381 381	0	0
4	G	30	Total O 30 30	0	0
4	H	29	Total O 29 29	0	0
4	I	29	Total O 29 29	0	0

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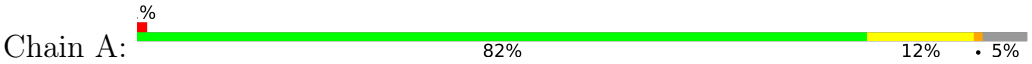
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	28	Total O 28 28	0	0
4	K	32	Total O 32 32	0	0
4	L	28	Total O 28 28	0	0

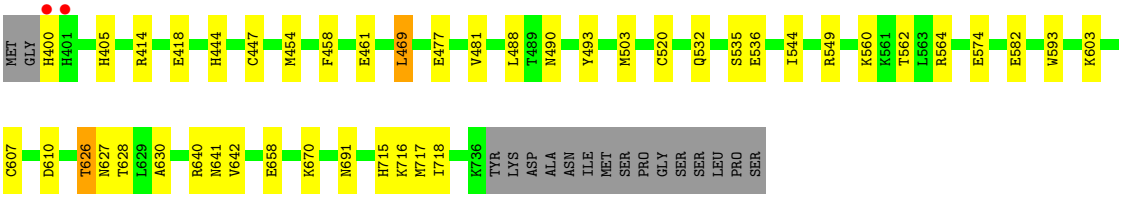
3 Residue-property plots

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: Adenomatous polyposis coli protein

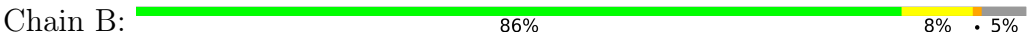
Chain A:

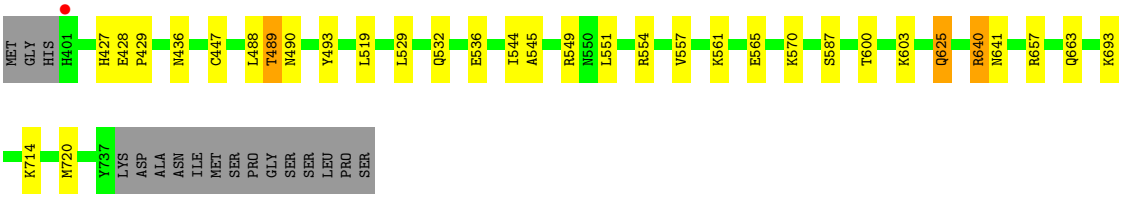




• Molecule 1: Adenomatous polyposis coli protein

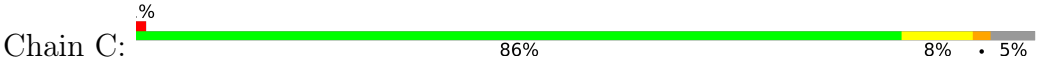
Chain B:

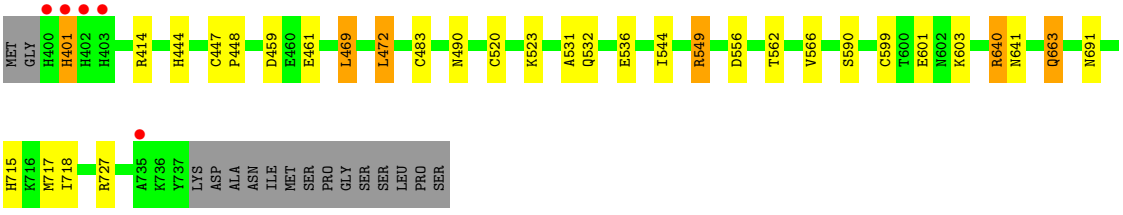




• Molecule 1: Adenomatous polyposis coli protein

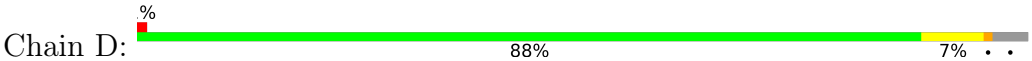
Chain C:

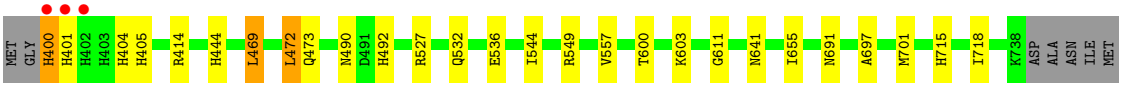




• Molecule 1: Adenomatous polyposis coli protein

Chain D:



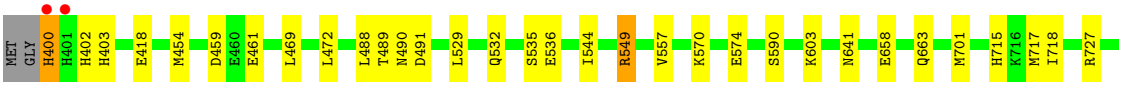


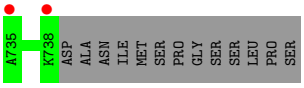
• Molecule 1: Adenomatous polyposis coli protein

Chain E:

• Molecule 1: Adenomatous polyposis coli protein

Chain F:





• Molecule 2: APC membrane recruitment protein 1

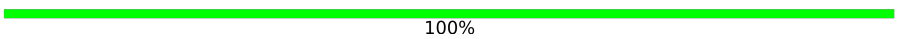
Chain G:

• Molecule 2: APC membrane recruitment protein 1

Chain H:

• Molecule 2: APC membrane recruitment protein 1

Chain I:



There are no outlier residues recorded for this chain.

• Molecule 2: APC membrane recruitment protein 1

Chain J:

• Molecule 2: APC membrane recruitment protein 1

Chain K:

• Molecule 2: APC membrane recruitment protein 1

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.59Å 168.93Å 170.27Å 60.29° 90.07° 90.05°	Depositor
Resolution (Å)	49.34 – 2.10 49.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.34-2.10) 98.0 (49.34-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.225 0.207 , 0.224	Depositor DCC
R_{free} test set	16980 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.328 for h,l,-k+l 0.328 for h,k-l,k 0.327 for h,-k+l,-k 0.327 for h,-l,k-l 0.438 for h,-k,-l 0.017 for -h,k,k-l 0.019 for -h,-k+l,l 0.015 for -h,l,k 0.015 for -h,-l,-k 0.017 for -h,-k,-k+l 0.018 for -h,k-l,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18962	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0/2668	0.50	0/3607
1	B	0.47	0/2659	0.52	1/3595 (0.0%)
1	C	0.47	0/2670	0.50	0/3610
1	D	0.45	0/2679	0.49	0/3621
1	E	0.44	0/2679	0.49	0/3621
1	F	0.43	0/2679	0.50	0/3621
2	G	0.43	0/121	0.63	0/160
2	H	0.43	0/111	0.57	0/147
2	I	0.41	0/111	0.57	0/147
2	J	0.44	0/111	0.55	0/147
2	K	0.39	0/111	0.55	0/147
2	L	0.44	0/111	0.54	0/147
All	All	0.45	0/16710	0.51	1/22570 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	436	ASN	C-N-CD	5.78	140.55	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2620	0	2626	38	0
1	B	2615	0	2621	21	0
1	C	2625	0	2628	24	0
1	D	2634	0	2641	24	0
1	E	2634	0	2641	29	0
1	F	2634	0	2641	24	0
2	G	115	0	99	1	0
2	H	108	0	90	1	0
2	I	108	0	90	0	0
2	J	108	0	90	2	0
2	K	108	0	90	2	0
2	L	108	0	90	0	0
3	A	36	0	54	9	0
3	B	20	0	30	1	0
3	C	20	0	30	6	0
3	D	28	0	42	8	0
3	E	28	0	42	1	0
3	F	16	0	24	2	0
4	A	378	0	0	5	0
4	B	347	0	0	3	0
4	C	367	0	0	4	0
4	D	381	0	0	5	0
4	E	367	0	0	6	0
4	F	381	0	0	3	0
4	G	30	0	0	0	0
4	H	29	0	0	0	0
4	I	29	0	0	0	0
4	J	28	0	0	0	0
4	K	32	0	0	0	0
4	L	28	0	0	1	0
All	All	18962	0	16569	156	0

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 5.

All (156) 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:D:611:GLY:H	3:D:805:EDO:H22	1.23	1.00
1:D:655:ILE:HD13	3:D:805:EDO:H12	1.54	0.87
1:D:697:ALA:O	1:D:701:MET:HG3	1.73	0.86
1:A:454:MET:HE2	1:A:458:PHE:HE2	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:CE	1:A:458:PHE:HE2	1.92	0.82
1:F:489:THR:HG22	1:F:491:ASP:H	1.45	0.80
1:B:561:LYS:HE3	1:B:565:GLU:OE1	1.83	0.79
1:F:489:THR:HB	4:F:1190:HOH:O	1.82	0.79
1:E:454:MET:HE1	1:E:455:LYS:HA	1.64	0.78
1:A:628:THR:HG22	1:A:630:ALA:H	1.50	0.76
1:B:561:LYS:CE	1:B:565:GLU:OE1	2.35	0.75
1:C:483:CYS:HB3	3:C:801:EDO:H12	1.70	0.72
1:D:691:ASN:HD22	3:D:804:EDO:C2	2.03	0.72
1:D:691:ASN:HD22	3:D:804:EDO:H21	1.56	0.71
1:F:549:ARG:HD3	1:F:590:SER:HB3	1.73	0.71
1:A:535:SER:HA	3:A:808:EDO:H12	1.74	0.69
1:C:459:ASP:OD2	1:C:461:GLU:HG2	1.96	0.66
1:C:691:ASN:HD22	3:C:803:EDO:H21	1.61	0.66
1:D:600:THR:HA	1:D:603:LYS:HD2	1.79	0.65
1:B:489:THR:HG21	4:B:1127:HOH:O	1.97	0.65
1:F:663:GLN:HG3	1:F:701:MET:SD	2.38	0.64
1:D:532:GLN:HB2	1:D:544:ILE:HG13	1.80	0.64
1:F:489:THR:CG2	1:F:491:ASP:H	2.11	0.63
1:C:640:ARG:NH1	2:H:497:ARG:O	2.31	0.63
1:E:454:MET:HE3	1:E:458:PHE:CE2	2.33	0.63
1:A:418:GLU:OE1	1:D:405:HIS:HD2	1.81	0.63
1:A:418:GLU:OE2	1:D:404:HIS:HD2	1.80	0.62
1:A:454:MET:CE	1:A:458:PHE:CE2	2.79	0.62
1:D:473:GLN:HE22	1:F:400:HIS:CD2	2.17	0.62
3:D:805:EDO:H11	4:D:1149:HOH:O	2.00	0.62
1:C:549:ARG:HD3	1:C:590:SER:HB3	1.81	0.62
1:A:454:MET:HE3	1:A:503:MET:HE1	1.82	0.61
1:C:532:GLN:HB2	1:C:544:ILE:HG13	1.83	0.61
1:D:611:GLY:N	3:D:805:EDO:H22	2.07	0.60
1:F:717:MET:HE1	4:L:601:HOH:O	2.00	0.60
1:F:489:THR:HG21	4:F:979:HOH:O	2.01	0.60
1:E:401:HIS:HB3	4:E:1186:HOH:O	2.02	0.59
1:B:625:GLN:HG3	4:B:1045:HOH:O	2.03	0.58
1:E:640:ARG:NH1	2:J:497:ARG:O	2.35	0.58
1:A:454:MET:HE2	1:A:458:PHE:CE2	2.34	0.57
1:B:532:GLN:HB2	1:B:544:ILE:HG13	1.85	0.57
1:B:603:LYS:HE3	1:B:641:ASN:O	2.04	0.57
1:F:715:HIS:HD2	1:F:718:ILE:H	1.50	0.57
1:E:715:HIS:HD2	1:E:718:ILE:H	1.52	0.57
1:A:670:LYS:HG2	3:A:805:EDO:H12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:GLN:HB2	1:E:544:ILE:HG13	1.87	0.56
1:A:405:HIS:HD2	1:F:418:GLU:OE1	1.89	0.56
1:E:454:MET:CE	1:E:455:LYS:HA	2.35	0.56
1:A:454:MET:HE1	1:A:458:PHE:CE2	2.41	0.56
1:E:454:MET:CE	1:E:458:PHE:CE2	2.89	0.56
1:F:532:GLN:HB2	1:F:544:ILE:HG13	1.88	0.55
1:D:400:HIS:N	1:D:400:HIS:CD2	2.73	0.55
1:D:490:ASN:ND2	1:D:536:GLU:OE2	2.33	0.55
1:F:570:LYS:O	1:F:574:GLU:HG3	2.07	0.55
1:C:490:ASN:ND2	1:C:536:GLU:OE2	2.38	0.55
1:C:603:LYS:HE3	1:C:641:ASN:O	2.06	0.54
1:B:488:LEU:C	3:B:803:EDO:H22	2.27	0.53
1:A:488:LEU:C	3:A:808:EDO:H11	2.29	0.53
1:B:554:ARG:NH2	1:F:658:GLU:OE1	2.41	0.53
1:F:402:HIS:CE1	1:F:403:HIS:ND1	2.77	0.53
1:D:715:HIS:HD2	1:D:718:ILE:H	1.54	0.53
1:B:657:ARG:CZ	1:B:693:LYS:HD3	2.39	0.52
1:E:490:ASN:ND2	1:E:536:GLU:OE1	2.40	0.52
1:A:715[A]:HIS:HD2	1:A:718:ILE:H	1.58	0.52
1:D:401:HIS:H	1:D:401:HIS:CD2	2.28	0.52
1:C:691:ASN:HD22	3:C:803:EDO:C2	2.22	0.52
1:B:600:THR:HA	1:B:603:LYS:HD2	1.91	0.52
1:C:531:ALA:HB3	3:C:801:EDO:H11	1.92	0.52
1:C:715:HIS:HD2	1:C:718:ILE:H	1.57	0.51
1:C:599:CYS:SG	1:C:601:GLU:HG2	2.51	0.51
1:A:454:MET:CE	1:A:503:MET:HE1	2.41	0.51
1:A:582:GLU:OE2	1:A:626:THR:HG22	2.11	0.51
1:F:488:LEU:C	3:F:803:EDO:H11	2.31	0.51
1:F:459:ASP:OD2	1:F:461:GLU:HG2	2.11	0.50
1:C:717:MET:HG3	4:C:1044:HOH:O	2.12	0.50
1:E:454:MET:HE3	1:E:458:PHE:HE2	1.75	0.50
1:E:658:GLU:OE2	4:E:901:HOH:O	2.20	0.49
1:E:697:ALA:HB1	1:E:701:MET:HE3	1.94	0.49
1:B:427:HIS:HE1	4:B:1128:HOH:O	1.95	0.49
1:A:603:LYS:HE3	1:A:641:ASN:O	2.12	0.49
1:A:691:ASN:HD22	3:A:807:EDO:H21	1.75	0.49
1:A:691:ASN:HD22	3:A:807:EDO:C2	2.25	0.49
1:A:658:GLU:OE1	4:A:1142:HOH:O	2.20	0.49
1:B:561:LYS:HE2	1:B:565:GLU:OE1	2.10	0.49
1:F:400:HIS:ND1	1:F:400:HIS:N	2.60	0.49
1:B:545:ALA:HB3	1:B:587:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLN:HB2	1:A:544:ILE:HG13	1.96	0.48
1:C:401:HIS:N	1:C:401:HIS:ND1	2.60	0.48
1:E:520:CYS:O	1:E:562:THR:HG21	2.14	0.48
1:C:727:ARG:NH2	4:C:999:HOH:O	2.44	0.47
1:A:520:CYS:O	1:A:562:THR:HG21	2.15	0.47
1:C:566:VAL:HA	3:C:804:EDO:H12	1.95	0.47
1:E:406:MET:HB2	3:E:806:EDO:H11	1.95	0.47
1:E:625:GLN:HG3	4:E:1128:HOH:O	2.15	0.47
1:A:454:MET:CE	1:A:503:MET:CE	2.93	0.47
1:E:444:HIS:HD2	4:E:1126:HOH:O	1.98	0.47
1:A:628:THR:HG21	4:A:1045:HOH:O	2.15	0.47
1:E:454:MET:CE	1:E:458:PHE:HE2	2.27	0.47
1:A:488:LEU:HB3	3:A:808:EDO:H11	1.97	0.46
1:E:454:MET:HE2	1:E:458:PHE:CD2	2.51	0.46
1:A:607:CYS:SG	1:A:642:VAL:HG13	2.56	0.46
1:A:414:ARG:NH2	1:A:469:LEU:O	2.48	0.46
1:C:447:CYS:HB3	1:C:448:PRO:HD3	1.97	0.46
1:F:529:LEU:O	1:F:544:ILE:HG21	2.16	0.46
1:A:626:THR:OG1	1:A:627:ASN:N	2.49	0.46
1:F:490:ASN:ND2	1:F:536:GLU:OE2	2.47	0.46
1:E:454:MET:CE	1:E:458:PHE:CD2	2.99	0.46
1:A:564:ARG:HD2	4:A:998:HOH:O	2.16	0.45
1:F:727:ARG:NH2	4:F:901:HOH:O	2.49	0.45
1:E:444:HIS:CD2	4:E:1126:HOH:O	2.69	0.45
1:E:454:MET:HE2	1:E:454:MET:O	2.16	0.45
1:B:490:ASN:ND2	1:B:536:GLU:OE2	2.47	0.45
1:D:472:LEU:HB3	3:D:806:EDO:H22	1.99	0.45
1:D:603:LYS:HE3	1:D:641:ASN:O	2.17	0.44
1:D:527:ARG:NH1	4:D:1213:HOH:O	2.50	0.44
1:E:406:MET:HE3	1:E:465:ALA:C	2.38	0.44
1:F:603:LYS:HE3	1:F:641:ASN:O	2.19	0.43
1:C:556:ASP:HB2	4:D:1007:HOH:O	2.18	0.43
1:D:444:HIS:HD2	4:D:1242:HOH:O	2.01	0.43
1:E:403:HIS:CE1	4:E:1129:HOH:O	2.70	0.43
4:A:1194:HOH:O	1:D:492:HIS:HD2	2.02	0.43
1:B:519:LEU:HD23	1:B:551:LEU:HD21	2.00	0.43
1:B:561:LYS:CE	1:B:565:GLU:CD	2.87	0.43
1:D:401:HIS:CD2	1:D:401:HIS:N	2.87	0.43
1:A:444:HIS:HE1	3:A:806:EDO:O1	2.02	0.42
1:A:447:CYS:HB2	1:A:493:TYR:CZ	2.53	0.42
1:F:535:SER:HA	3:F:803:EDO:H12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:CYS:SG	1:E:601:GLU:HG2	2.59	0.42
1:C:472:LEU:HB3	3:C:802:EDO:H11	2.01	0.42
1:A:454:MET:HE2	1:A:503:MET:HE2	2.02	0.42
1:A:536:GLU:H	3:A:808:EDO:C2	2.33	0.42
1:B:447:CYS:HB2	1:B:493:TYR:CZ	2.54	0.42
1:C:444:HIS:HE1	4:C:1164:HOH:O	2.02	0.42
1:A:560:LYS:NZ	4:A:1221:HOH:O	2.52	0.42
1:C:520:CYS:O	1:C:562:THR:HG21	2.19	0.42
1:E:406:MET:CE	1:E:465:ALA:HB1	2.49	0.42
1:E:414:ARG:NH2	1:E:469:LEU:O	2.49	0.42
1:E:625:GLN:HG3	1:E:625:GLN:H	1.70	0.42
1:E:406:MET:HE1	1:E:465:ALA:HB1	2.02	0.42
1:F:402:HIS:ND1	1:F:403:HIS:ND1	2.68	0.42
1:A:593:TRP:CE3	2:G:501:SER:HB3	2.55	0.41
1:B:640:ARG:HH12	2:K:496:PRO:HB2	1.85	0.41
1:E:406:MET:HB3	1:E:406:MET:HE2	1.84	0.41
1:B:529:LEU:O	1:B:544:ILE:HG21	2.20	0.41
1:F:549:ARG:CD	1:F:590:SER:HB3	2.47	0.41
1:C:663:GLN:HG3	4:C:1134:HOH:O	2.21	0.41
1:C:523:LYS:HE2	1:C:562:THR:OG1	2.21	0.41
1:A:477:GLU:O	1:A:481:VAL:HG13	2.21	0.41
1:B:428:GLU:HG3	1:B:429:PRO:HD2	2.02	0.41
1:A:490:ASN:OD1	3:A:808:EDO:H22	2.21	0.40
1:D:414:ARG:NH2	1:D:469:LEU:O	2.52	0.40
1:D:691:ASN:HD22	3:D:804:EDO:H22	1.84	0.40
1:C:414:ARG:NH2	1:C:469:LEU:O	2.51	0.40
1:A:610:ASP:HB3	2:J:497:ARG:NE	2.37	0.40
1:B:640:ARG:NH1	2:K:497:ARG:O	2.55	0.40
1:D:444:HIS:CD2	4:D:1242:HOH:O	2.74	0.40

There are no symmetry-related clashes.

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	336/354 (95%)	330 (98%)	6 (2%)	0	100	100
1	B	335/354 (95%)	331 (99%)	4 (1%)	0	100	100
1	C	336/354 (95%)	333 (99%)	3 (1%)	0	100	100
1	D	337/354 (95%)	331 (98%)	6 (2%)	0	100	100
1	E	337/354 (95%)	334 (99%)	3 (1%)	0	100	100
1	F	337/354 (95%)	334 (99%)	3 (1%)	0	100	100
2	G	11/13 (85%)	11 (100%)	0	0	100	100
2	H	11/13 (85%)	11 (100%)	0	0	100	100
2	I	11/13 (85%)	11 (100%)	0	0	100	100
2	J	11/13 (85%)	11 (100%)	0	0	100	100
2	K	11/13 (85%)	11 (100%)	0	0	100	100
2	L	11/13 (85%)	11 (100%)	0	0	100	100
All	All	2084/2202 (95%)	2059 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	287/300 (96%)	278 (97%)	9 (3%)	40	43
1	B	286/300 (95%)	277 (97%)	9 (3%)	40	43
1	C	287/300 (96%)	281 (98%)	6 (2%)	53	59
1	D	288/300 (96%)	283 (98%)	5 (2%)	60	67
1	E	288/300 (96%)	280 (97%)	8 (3%)	43	47
1	F	288/300 (96%)	282 (98%)	6 (2%)	53	59
2	G	12/11 (109%)	12 (100%)	0	100	100
2	H	11/11 (100%)	11 (100%)	0	100	100
2	I	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	11/11 (100%)	11 (100%)	0	100 100
2	K	11/11 (100%)	11 (100%)	0	100 100
2	L	11/11 (100%)	10 (91%)	1 (9%)	9 6
All	All	1791/1866 (96%)	1747 (98%)	44 (2%)	47 52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	HIS
1	A	461	GLU
1	A	469	LEU
1	A	549	ARG
1	A	574	GLU
1	A	626	THR
1	A	640	ARG
1	A	716	LYS
1	A	717	MET
1	B	489	THR
1	B	549	ARG
1	B	557	VAL
1	B	570	LYS
1	B	625	GLN
1	B	640	ARG
1	B	663	GLN
1	B	714	LYS
1	B	720	MET
1	C	401	HIS
1	C	469	LEU
1	C	472	LEU
1	C	549	ARG
1	C	640	ARG
1	C	663	GLN
1	D	400	HIS
1	D	469	LEU
1	D	472	LEU
1	D	549	ARG
1	D	557	VAL
1	E	428	GLU
1	E	454	MET
1	E	469	LEU
1	E	557	VAL

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Mol	Chain	Res	Type
1	E	625	GLN
1	E	627	ASN
1	E	663	GLN
1	E	738	LYS
1	F	400	HIS
1	F	454	MET
1	F	469	LEU
1	F	472	LEU
1	F	549	ARG
1	F	557	VAL
2	L	507	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	HIS
1	A	405	HIS
1	A	424	GLN
1	A	444	HIS
1	A	558	ASN
1	A	695	GLN
1	A	709	ASN
1	A	732	ASN
1	B	412	GLN
1	B	424	GLN
1	B	444	HIS
1	B	659	ASN
1	B	663	GLN
1	B	667	GLN
1	B	695	GLN
1	B	709	ASN
1	B	715	HIS
1	B	732	ASN
1	C	403	HIS
1	C	412	GLN
1	C	424	GLN
1	C	444	HIS
1	C	445	GLN
1	C	695	GLN
1	C	709	ASN
1	C	715	HIS
1	D	400	HIS

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Mol	Chain	Res	Type
1	D	401	HIS
1	D	403	HIS
1	D	404	HIS
1	D	405	HIS
1	D	424	GLN
1	D	444	HIS
1	D	667	GLN
1	D	691	ASN
1	D	695	GLN
1	D	709	ASN
1	D	715	HIS
1	D	732	ASN
1	E	400	HIS
1	E	412	GLN
1	E	444	HIS
1	E	445	GLN
1	E	627	ASN
1	E	659	ASN
1	E	695	GLN
1	E	709	ASN
1	E	715	HIS
1	F	400	HIS
1	F	424	GLN
1	F	444	HIS
1	F	445	GLN
1	F	667	GLN
1	F	695	GLN
1	F	709	ASN
1	F	715	HIS
1	F	732	ASN

5.3.3 RNA (i)

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)

37 ligands are modelled in this entry.

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	EDO	C	805	-	3,3,3	0.47	0	2,2,2	0.18	0
3	EDO	B	805	-	3,3,3	0.42	0	2,2,2	0.33	0
3	EDO	E	805	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	F	801	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	D	802	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	A	809	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	E	806	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	A	803	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	A	804	-	3,3,3	0.50	0	2,2,2	0.22	0
3	EDO	B	801	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	F	802	-	3,3,3	0.48	0	2,2,2	0.30	0
3	EDO	C	801	-	3,3,3	0.55	0	2,2,2	0.31	0
3	EDO	A	805	-	3,3,3	0.42	0	2,2,2	0.61	0
3	EDO	C	803	-	3,3,3	0.48	0	2,2,2	0.17	0
3	EDO	B	803	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	D	801	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	B	804	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	807	-	3,3,3	0.46	0	2,2,2	0.21	0
3	EDO	E	807	-	3,3,3	0.46	0	2,2,2	0.39	0
3	EDO	D	807	-	3,3,3	0.46	0	2,2,2	0.43	0
3	EDO	F	803	-	3,3,3	0.42	0	2,2,2	0.21	0
3	EDO	D	804	-	3,3,3	0.47	0	2,2,2	0.20	0
3	EDO	A	802	-	3,3,3	0.54	0	2,2,2	0.21	0
3	EDO	E	801	-	3,3,3	0.48	0	2,2,2	0.17	0
3	EDO	E	802	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	D	806	-	3,3,3	0.54	0	2,2,2	0.16	0
3	EDO	A	808	-	3,3,3	0.39	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	E	804	-	3,3,3	0.47	0	2,2,2	0.45	0
3	EDO	A	801	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	A	806	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	C	802	-	3,3,3	0.52	0	2,2,2	0.12	0
3	EDO	B	802	-	3,3,3	0.46	0	2,2,2	0.25	0
3	EDO	C	804	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	E	803	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	D	803	-	3,3,3	0.47	0	2,2,2	0.15	0
3	EDO	F	804	-	3,3,3	0.55	0	2,2,2	0.09	0
3	EDO	D	805	-	3,3,3	0.48	0	2,2,2	0.42	0

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	EDO	C	805	-	-	0/1/1/1	-
3	EDO	B	805	-	-	1/1/1/1	-
3	EDO	E	805	-	-	0/1/1/1	-
3	EDO	F	801	-	-	0/1/1/1	-
3	EDO	D	802	-	-	1/1/1/1	-
3	EDO	A	809	-	-	0/1/1/1	-
3	EDO	E	806	-	-	0/1/1/1	-
3	EDO	A	803	-	-	1/1/1/1	-
3	EDO	A	804	-	-	1/1/1/1	-
3	EDO	B	801	-	-	1/1/1/1	-
3	EDO	F	802	-	-	1/1/1/1	-
3	EDO	C	801	-	-	1/1/1/1	-
3	EDO	A	805	-	-	1/1/1/1	-
3	EDO	C	803	-	-	0/1/1/1	-
3	EDO	B	803	-	-	1/1/1/1	-
3	EDO	D	801	-	-	1/1/1/1	-
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	A	807	-	-	0/1/1/1	-
3	EDO	E	807	-	-	1/1/1/1	-
3	EDO	D	807	-	-	1/1/1/1	-
3	EDO	F	803	-	-	1/1/1/1	-
3	EDO	D	804	-	-	1/1/1/1	-
3	EDO	A	802	-	-	1/1/1/1	-
3	EDO	E	801	-	-	0/1/1/1	-
3	EDO	E	802	-	-	0/1/1/1	-
3	EDO	D	806	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	808	-	-	0/1/1/1	-
3	EDO	E	804	-	-	1/1/1/1	-
3	EDO	A	801	-	-	0/1/1/1	-
3	EDO	A	806	-	-	1/1/1/1	-
3	EDO	C	802	-	-	0/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
3	EDO	C	804	-	-	1/1/1/1	-
3	EDO	E	803	-	-	0/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	F	804	-	-	0/1/1/1	-
3	EDO	D	805	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	805	EDO	O1-C1-C2-O2
3	A	804	EDO	O1-C1-C2-O2
3	A	806	EDO	O1-C1-C2-O2
3	D	805	EDO	O1-C1-C2-O2
3	C	804	EDO	O1-C1-C2-O2
3	F	802	EDO	O1-C1-C2-O2
3	C	801	EDO	O1-C1-C2-O2
3	D	807	EDO	O1-C1-C2-O2
3	A	803	EDO	O1-C1-C2-O2
3	B	805	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2
3	E	804	EDO	O1-C1-C2-O2
3	B	803	EDO	O1-C1-C2-O2
3	B	801	EDO	O1-C1-C2-O2
3	D	801	EDO	O1-C1-C2-O2
3	D	804	EDO	O1-C1-C2-O2
3	D	806	EDO	O1-C1-C2-O2
3	E	807	EDO	O1-C1-C2-O2
3	F	803	EDO	O1-C1-C2-O2
3	A	802	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	806	EDO	1	0
3	C	801	EDO	2	0
3	A	805	EDO	1	0
3	C	803	EDO	2	0
3	B	803	EDO	1	0
3	A	807	EDO	2	0
3	F	803	EDO	2	0
3	D	804	EDO	3	0
3	D	806	EDO	1	0
3	A	808	EDO	5	0
3	A	806	EDO	1	0
3	C	802	EDO	1	0
3	C	804	EDO	1	0
3	D	805	EDO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	337/354 (95%)	-0.24	2 (0%) 89 91	13, 22, 41, 58	22 (6%)
1	B	337/354 (95%)	-0.30	1 (0%) 94 94	12, 22, 40, 60	19 (5%)
1	C	338/354 (95%)	-0.23	5 (1%) 73 77	12, 23, 41, 62	22 (6%)
1	D	339/354 (95%)	-0.29	3 (0%) 84 86	12, 23, 41, 71	19 (5%)
1	E	339/354 (95%)	-0.29	0 100 100	13, 22, 41, 71	15 (4%)
1	F	339/354 (95%)	-0.29	4 (1%) 79 82	12, 22, 40, 71	17 (5%)
2	G	13/13 (100%)	0.04	0 100 100	20, 27, 38, 48	1 (7%)
2	H	13/13 (100%)	-0.13	0 100 100	21, 25, 36, 54	1 (7%)
2	I	13/13 (100%)	-0.05	0 100 100	22, 26, 38, 56	1 (7%)
2	J	13/13 (100%)	-0.11	0 100 100	21, 25, 40, 57	1 (7%)
2	K	13/13 (100%)	0.01	0 100 100	21, 26, 38, 63	1 (7%)
2	L	13/13 (100%)	-0.27	0 100 100	19, 23, 38, 52	1 (7%)
All	All	2107/2202 (95%)	-0.26	15 (0%) 87 89	12, 23, 41, 71	120 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	HIS	4.4
1	D	401	HIS	4.2
1	B	401	HIS	3.2
1	A	401	HIS	2.9
1	C	735	ALA	2.8
1	F	735	ALA	2.8
1	D	402	HIS	2.7
1	F	738	LYS	2.7
1	A	400	HIS	2.5
1	F	401	HIS	2.5
1	C	400	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	402	HIS	2.2
1	D	400	HIS	2.1
1	F	400	HIS	2.1
1	C	403	HIS	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 (i)

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, 95^{th} 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	EDO	C	803	4/4	0.67	0.14	43,43,44,44	0
3	EDO	D	804	4/4	0.77	0.13	42,42,42,43	0
3	EDO	A	808	4/4	0.80	0.15	40,40,41,41	0
3	EDO	A	804	4/4	0.83	0.16	37,40,41,43	0
3	EDO	F	801	4/4	0.83	0.12	34,38,39,41	0
3	EDO	B	804	4/4	0.86	0.27	33,35,35,38	0
3	EDO	E	804	4/4	0.87	0.12	43,44,44,44	0
3	EDO	C	804	4/4	0.88	0.16	39,41,41,42	0
3	EDO	A	806	4/4	0.88	0.10	39,40,40,42	0
3	EDO	E	803	4/4	0.88	0.16	30,32,33,33	0
3	EDO	C	801	4/4	0.88	0.13	23,28,28,33	0
3	EDO	B	803	4/4	0.88	0.18	38,39,40,40	0
3	EDO	A	803	4/4	0.90	0.13	32,34,36,37	0
3	EDO	D	802	4/4	0.91	0.17	35,35,37,37	0
3	EDO	B	805	4/4	0.91	0.08	42,42,42,43	0
3	EDO	D	806	4/4	0.91	0.13	24,24,25,26	0
3	EDO	D	807	4/4	0.92	0.10	45,46,47,48	0
3	EDO	E	806	4/4	0.92	0.21	33,34,35,36	0
3	EDO	D	803	4/4	0.92	0.10	32,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	F	802	4/4	0.92	0.10	35,37,38,38	0
3	EDO	A	807	4/4	0.93	0.12	43,43,44,45	0
3	EDO	B	802	4/4	0.93	0.10	32,34,35,35	0
3	EDO	F	803	4/4	0.93	0.23	42,43,43,44	0
3	EDO	F	804	4/4	0.93	0.12	24,26,27,27	0
3	EDO	A	809	4/4	0.94	0.14	45,46,46,46	0
3	EDO	E	807	4/4	0.94	0.11	43,43,44,44	0
3	EDO	D	805	4/4	0.94	0.18	26,29,29,30	0
3	EDO	A	805	4/4	0.95	0.15	42,43,43,43	0
3	EDO	E	805	4/4	0.95	0.22	24,28,29,29	0
3	EDO	E	802	4/4	0.95	0.15	31,32,32,32	0
3	EDO	B	801	4/4	0.95	0.12	22,25,27,28	0
3	EDO	D	801	4/4	0.96	0.10	21,24,24,25	0
3	EDO	E	801	4/4	0.96	0.08	24,27,28,28	0
3	EDO	A	802	4/4	0.96	0.15	25,28,29,30	0
3	EDO	C	805	4/4	0.96	0.08	28,28,28,28	0
3	EDO	C	802	4/4	0.97	0.09	24,25,26,26	0
3	EDO	A	801	4/4	0.97	0.09	27,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.