Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 04:19 pm BST

PDB ID	:	5EM2
Title	:	Crystal structure of the Erb1-Ytm1 complex
Authors	:	Ahmed, Y.L.; Sinning, I.
Deposited on	:	2015-11-05
Resolution	:	2.67 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 (i) 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 (i)) were used in the production of this report:

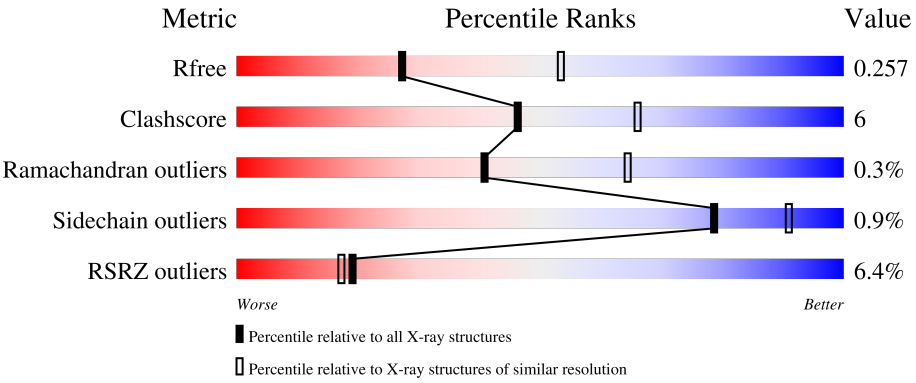
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	388	2% 81% 11% 8%
1	C	388	2% 82% 10% 8%
2	B	499	8% 75% 17% 8%
2	D	499	10% 72% 19% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12754 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 Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2804	1786	514	498	6			
1	C	357	Total	C	N	O	S	0	0	0
			2804	1786	514	498	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	414	MET	-	initiating methionine	UNP G0SCK6
A	415	ALA	-	expression tag	UNP G0SCK6
A	416	HIS	-	expression tag	UNP G0SCK6
A	417	HIS	-	expression tag	UNP G0SCK6
A	418	HIS	-	expression tag	UNP G0SCK6
A	419	HIS	-	expression tag	UNP G0SCK6
A	420	HIS	-	expression tag	UNP G0SCK6
A	421	HIS	-	expression tag	UNP G0SCK6
A	422	MET	-	expression tag	UNP G0SCK6
C	414	MET	-	initiating methionine	UNP G0SCK6
C	415	ALA	-	expression tag	UNP G0SCK6
C	416	HIS	-	expression tag	UNP G0SCK6
C	417	HIS	-	expression tag	UNP G0SCK6
C	418	HIS	-	expression tag	UNP G0SCK6
C	419	HIS	-	expression tag	UNP G0SCK6
C	420	HIS	-	expression tag	UNP G0SCK6
C	421	HIS	-	expression tag	UNP G0SCK6
C	422	MET	-	expression tag	UNP G0SCK6

- Molecule 2 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	460	Total	C	N	O	S	0	0	0
			3469	2174	610	679	6			

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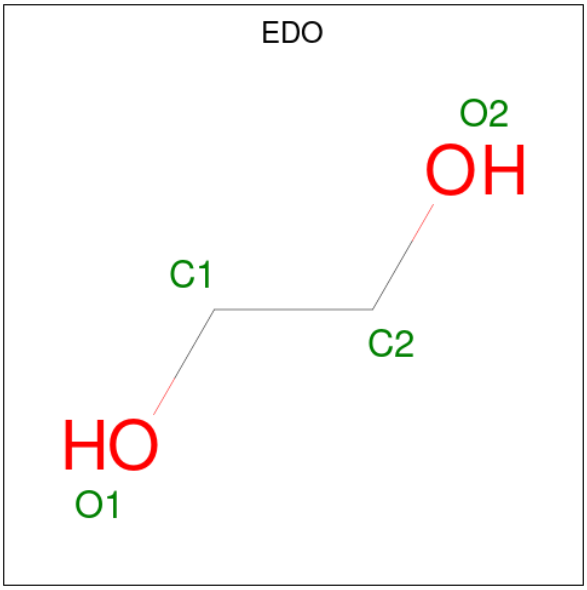
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	457	Total	C	N	O	S	0	0	0
			3449	2163	607	673	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP G0SFB5
B	-2	GLY	-	expression tag	UNP G0SFB5
B	-1	ALA	-	expression tag	UNP G0SFB5
B	0	HIS	-	expression tag	UNP G0SFB5
D	-3	GLY	-	expression tag	UNP G0SFB5
D	-2	GLY	-	expression tag	UNP G0SFB5
D	-1	ALA	-	expression tag	UNP G0SFB5
D	0	HIS	-	expression tag	UNP G0SFB5

- 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	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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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	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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is water.

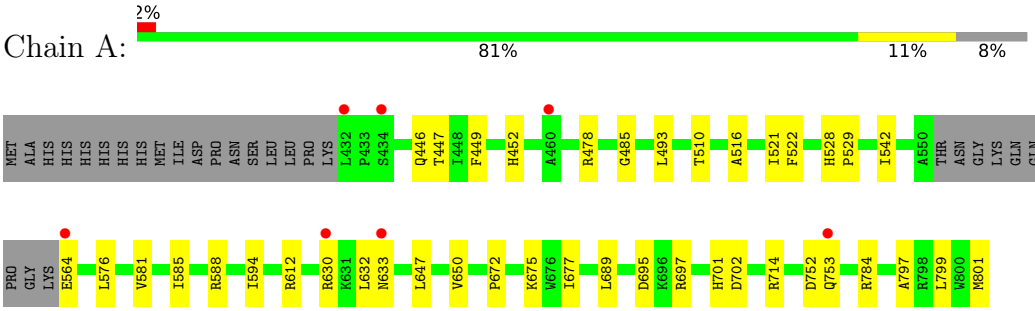
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	30	Total O 30 30	0	0
5	C	57	Total O 57 57	0	0
5	D	31	Total O 31 31	0	0

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.

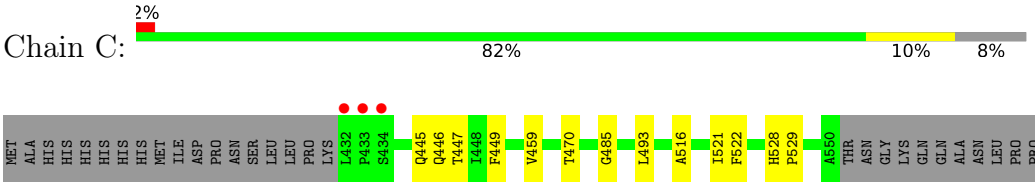
• Molecule 1: Ribosome biogenesis protein ERB1

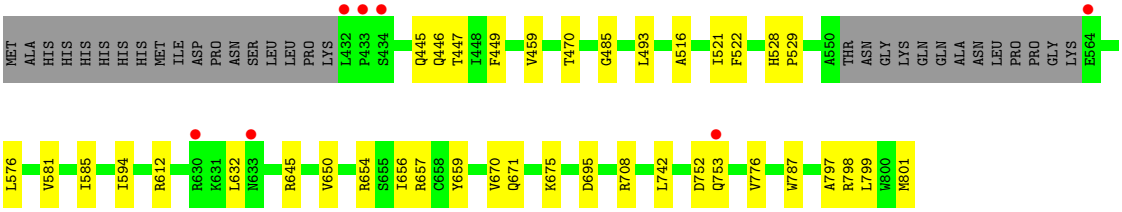
Chain A:



• Molecule 1: Ribosome biogenesis protein ERB1

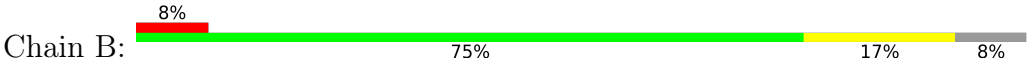
Chain C:

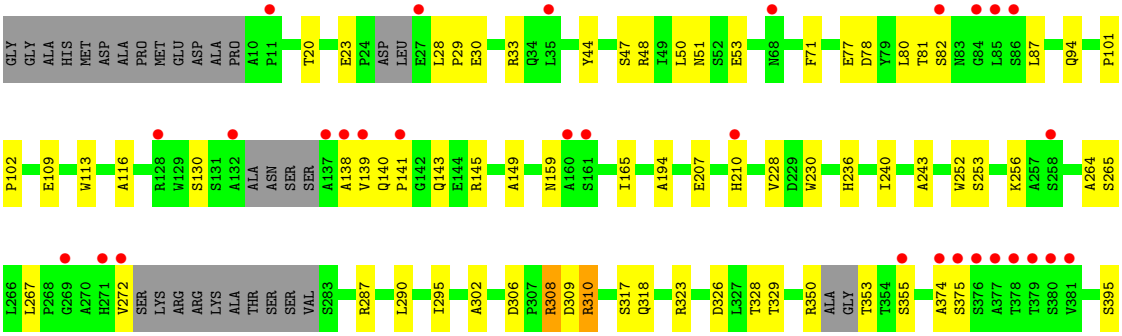


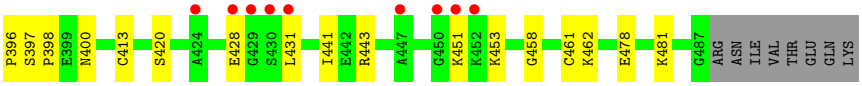


• Molecule 2: Ribosome biogenesis protein YTM1

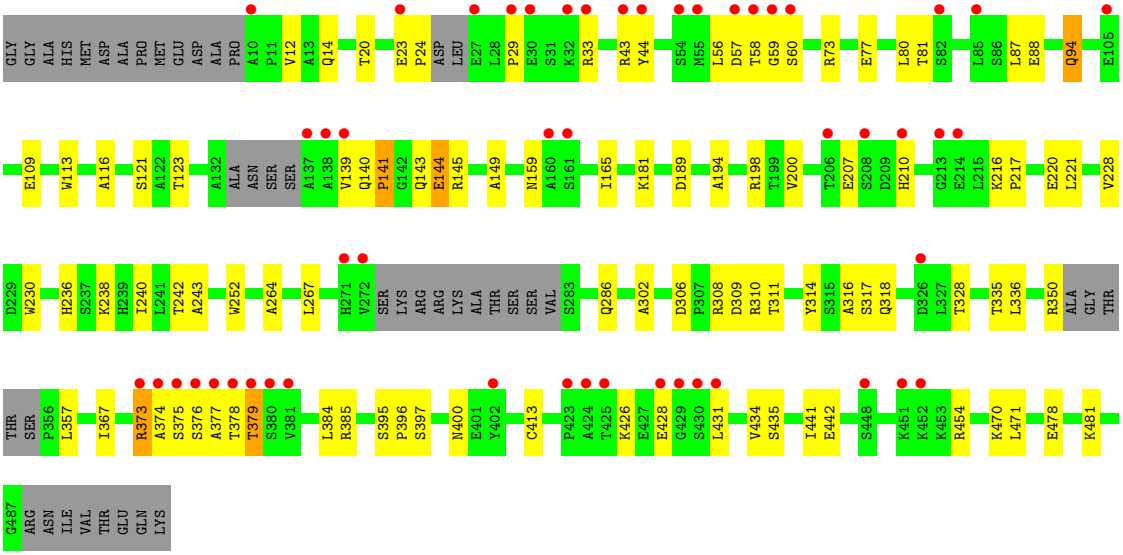
Chain B:







• Molecule 2: Ribosome biogenesis protein YTM1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.66Å 81.35Å 141.69Å 90.00° 100.23° 90.00°	Depositor
Resolution (Å)	48.61 – 2.67 48.61 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-2.67) 99.7 (48.61-2.67)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.69Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.221 , 0.251 0.231 , 0.257	Depositor DCC
R_{free} test set	2866 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12754	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.39% 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: MG, 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	0.22	0/2880	0.47	0/3917
1	C	0.22	0/2880	0.45	0/3917
2	B	0.24	0/3544	0.48	0/4825
2	D	0.25	0/3524	0.51	0/4796
All	All	0.23	0/12828	0.48	0/17455

There are no bond length outliers.

There are no bond angle outliers.

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	2804	0	2808	23	0
1	C	2804	0	2808	23	1
2	B	3469	0	3430	57	0
2	D	3449	0	3412	55	1
3	A	24	0	36	1	0
3	C	8	0	12	0	0
3	D	12	0	18	1	0
4	A	1	0	0	0	0
5	A	65	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	30	0	0	0	0
5	C	57	0	0	0	0
5	D	31	0	0	1	0
All	All	12754	0	12524	157	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 (157) 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)
2:B:428:GLU:HG3	2:B:431:LEU:HB2	1.65	0.78
2:D:236:HIS:HB3	2:D:310:ARG:HH22	1.51	0.76
1:A:632:LEU:HD11	1:A:650:VAL:HG11	1.73	0.71
1:A:675:LYS:N	1:A:695:ASP:OD2	2.23	0.71
1:A:564:GLU:O	1:A:588:ARG:NH2	2.25	0.70
2:D:336:LEU:HD12	2:D:376:SER:H	1.58	0.68
1:C:675:LYS:N	1:C:695:ASP:OD2	2.27	0.68
2:B:80:LEU:HD13	2:B:87:LEU:HA	1.77	0.67
2:B:159:ASN:HB3	2:B:165:ILE:HD11	1.76	0.66
2:B:451:LYS:HG3	2:B:453:LYS:H	1.58	0.66
2:B:236:HIS:HB3	2:B:310:ARG:HH12	1.61	0.65
1:A:702:ASP:OD2	1:C:645:ARG:NH2	2.31	0.64
2:D:336:LEU:HD12	2:D:376:SER:N	2.13	0.64
2:B:451:LYS:HE3	2:B:453:LYS:HB3	1.80	0.63
2:D:350:ARG:HD3	2:D:357:LEU:HB2	1.83	0.60
1:A:516:ALA:HB2	1:A:594:ILE:HD11	1.84	0.60
1:A:447:THR:HB	1:A:799:LEU:HB3	1.84	0.60
2:D:159:ASN:HB3	2:D:165:ILE:HD11	1.83	0.59
2:D:109:GLU:OE1	2:D:481:LYS:NZ	2.33	0.59
1:A:752:ASP:HB2	1:A:753:GLN:OE1	2.02	0.59
2:D:428:GLU:OE1	2:D:431:LEU:HB2	2.03	0.58
2:D:80:LEU:HD13	2:D:87:LEU:HA	1.84	0.58
2:D:145:ARG:NH2	2:D:207:GLU:OE1	2.28	0.58
2:D:426:LYS:HA	2:D:426:LYS:HE3	1.86	0.58
2:B:240:ILE:HB	2:B:252:TRP:HB2	1.86	0.58
2:B:265:SER:HB2	2:B:272:VAL:HG11	1.84	0.57
1:C:516:ALA:HB2	1:C:594:ILE:HD11	1.86	0.57
2:B:145:ARG:NH2	2:B:207:GLU:OE1	2.33	0.57
2:D:378:THR:OG1	2:D:379:THR:N	2.33	0.56
2:B:256:LYS:HE3	2:B:287:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LYS:HE3	2:B:287:ARG:HH11	1.71	0.55
2:D:210:HIS:N	2:D:210:HIS:CD2	2.73	0.55
2:B:397:SER:HB3	2:B:400:ASN:O	2.08	0.54
2:D:123:THR:HG21	2:D:470:LYS:HD2	1.90	0.54
2:B:77:GLU:HA	2:B:80:LEU:HD12	1.89	0.53
2:B:306:ASP:HB3	2:B:309:ASP:O	2.06	0.53
2:D:116:ALA:HB3	2:D:149:ALA:HB3	1.90	0.53
2:D:413:CYS:HB2	2:D:441:ILE:HB	1.89	0.53
1:C:447:THR:HB	1:C:799:LEU:HB3	1.91	0.53
2:D:306:ASP:HB3	2:D:309:ASP:O	2.09	0.53
2:B:109:GLU:OE2	2:B:481:LYS:NZ	2.42	0.52
2:B:113:TRP:CE2	2:B:478:GLU:HG3	2.44	0.52
1:C:656:ILE:HB	1:C:670:VAL:HB	1.91	0.52
2:B:78:ASP:O	2:B:82:SER:OG	2.19	0.52
2:B:30:GLU:HA	2:B:33:ARG:HG3	1.90	0.52
1:C:528:HIS:CD2	1:C:529:PRO:HD2	2.44	0.52
2:D:198:ARG:NH1	5:D:601:HOH:O	2.39	0.52
2:D:240:ILE:HB	2:D:252:TRP:HB2	1.91	0.51
2:D:43:ARG:NH2	2:D:73:ARG:HH11	2.08	0.51
1:A:647:LEU:HD13	3:A:906:EDO:H21	1.92	0.51
2:B:116:ALA:HB3	2:B:149:ALA:HB3	1.93	0.51
2:B:253:SER:HB2	2:B:290:LEU:HD11	1.92	0.50
2:D:335:THR:O	2:D:375:SER:HB2	2.11	0.50
1:A:697:ARG:NH2	1:A:714:ARG:HH12	2.08	0.50
2:B:28:LEU:HD12	2:B:29:PRO:HD2	1.94	0.50
2:B:23:GLU:OE1	2:B:23:GLU:N	2.45	0.50
2:D:236:HIS:O	2:D:238:LYS:NZ	2.44	0.49
1:C:449:PHE:HB2	1:C:797:ALA:HB3	1.94	0.49
2:D:113:TRP:CE2	2:D:478:GLU:HG3	2.48	0.49
2:D:230:TRP:HB3	2:D:243:ALA:HB3	1.96	0.48
2:B:326:ASP:OD1	2:B:328:THR:HG22	2.15	0.47
2:B:140:GLN:OE1	2:B:140:GLN:N	2.47	0.47
1:A:521:ILE:HD12	1:A:585:ILE:HB	1.97	0.47
2:B:94:GLN:O	2:B:94:GLN:HG3	2.14	0.47
2:D:58:THR:O	2:D:60:SER:N	2.44	0.46
2:B:130:SER:HB3	2:B:138:ALA:O	2.16	0.46
2:D:56:LEU:HD23	2:D:57:ASP:N	2.31	0.46
2:D:20:THR:O	2:D:94:GLN:HA	2.15	0.46
2:D:121:SER:HA	2:D:144:GLU:HB3	1.96	0.46
1:C:657:ARG:NH1	1:C:659:TYR:OH	2.46	0.46
1:C:632:LEU:HD21	1:C:650:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:TRP:HB3	2:B:243:ALA:HB3	1.97	0.46
2:B:53:GLU:H	2:B:53:GLU:CD	2.15	0.46
1:C:521:ILE:HD12	1:C:585:ILE:HB	1.98	0.46
2:B:353:THR:HG22	2:B:353:THR:O	2.15	0.45
2:D:181:LYS:NZ	3:D:501:EDO:O1	2.48	0.45
2:D:216:LYS:HA	2:D:217:PRO:HD3	1.83	0.45
2:B:317:SER:OG	2:B:318:GLN:N	2.49	0.45
2:B:413:CYS:HB2	2:B:441:ILE:HB	1.98	0.45
2:B:458:GLY:O	2:B:462:LYS:HG3	2.17	0.45
1:C:612:ARG:HG3	1:C:612:ARG:HH11	1.81	0.45
2:D:314:TYR:OH	2:D:373:ARG:NH2	2.50	0.45
2:B:308:ARG:HG2	2:B:353:THR:HG23	1.99	0.45
2:D:317:SER:OG	2:D:318:GLN:N	2.50	0.45
1:A:528:HIS:CD2	1:A:529:PRO:HD2	2.52	0.45
2:D:12:VAL:O	2:D:14:GLN:HG3	2.17	0.45
2:B:397:SER:HA	2:B:398:PRO:HD3	1.82	0.45
1:C:493:LEU:HD13	1:C:522:PHE:CD1	2.51	0.44
1:A:449:PHE:CE2	1:A:485:GLY:HA2	2.52	0.44
2:B:48:ARG:HA	2:B:51:ASN:HB2	1.99	0.44
2:D:77:GLU:O	2:D:81:THR:HG23	2.18	0.44
2:B:143:GLN:OE1	2:B:210:HIS:CG	2.69	0.44
2:B:71:PHE:HE2	2:B:420:SER:HB2	1.83	0.44
2:B:77:GLU:O	2:B:81:THR:HG23	2.16	0.44
2:D:140:GLN:HA	2:D:141:PRO:HD3	1.77	0.44
2:D:140:GLN:N	2:D:140:GLN:OE1	2.51	0.44
1:A:493:LEU:HD13	1:A:522:PHE:CD1	2.53	0.44
2:D:384:LEU:HD22	2:D:435:SER:HB3	1.99	0.44
1:C:446:GLN:HG3	1:C:801:MET:CG	2.48	0.43
2:B:101:PRO:HA	2:B:102:PRO:HD3	1.95	0.43
2:B:395:SER:HA	2:B:396:PRO:HD3	1.87	0.43
2:D:230:TRP:CG	2:D:302:ALA:HA	2.53	0.43
1:A:452:HIS:CD2	1:A:478:ARG:HD2	2.54	0.43
1:C:742:LEU:HD21	1:C:776:VAL:HG11	2.01	0.43
1:A:753:GLN:OE1	1:A:753:GLN:N	2.51	0.43
1:A:784:ARG:NH1	5:A:1004:HOH:O	2.40	0.43
2:B:194:ALA:HB1	2:B:228:VAL:HB	2.00	0.43
2:D:221:LEU:HB3	2:D:252:TRP:CZ3	2.53	0.43
1:C:675:LYS:HE2	1:C:675:LYS:HB3	1.77	0.43
1:A:446:GLN:HG3	1:A:801:MET:CG	2.49	0.42
1:A:449:PHE:HB2	1:A:797:ALA:HB3	2.01	0.42
2:D:395:SER:HA	2:D:396:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:TYR:CZ	2:B:48:ARG:HD2	2.53	0.42
1:A:612:ARG:HB3	1:A:630:ARG:NE	2.34	0.42
2:B:230:TRP:CG	2:B:302:ALA:HA	2.54	0.42
2:D:144:GLU:HG3	2:D:471:LEU:HD22	2.01	0.42
2:D:194:ALA:HB1	2:D:228:VAL:HB	2.02	0.42
2:B:44:TYR:O	2:B:48:ARG:HG3	2.18	0.42
2:B:374:ALA:O	2:B:375:SER:HB2	2.19	0.42
2:D:302:ALA:HB3	2:D:316:ALA:HB3	2.01	0.42
1:C:445:GLN:OE1	1:C:798:ARG:NH1	2.44	0.42
2:D:367:ILE:HB	2:D:384:LEU:HB2	2.02	0.42
2:D:397:SER:HB3	2:D:400:ASN:O	2.20	0.42
1:C:752:ASP:HB2	1:C:753:GLN:OE1	2.20	0.42
2:D:377:ALA:O	2:D:379:THR:HG23	2.20	0.42
1:C:671:GLN:O	1:C:708:ARG:HD3	2.21	0.41
2:B:295:ILE:HD12	2:B:323:ARG:HD2	2.02	0.41
1:C:576:LEU:HB3	1:C:581:VAL:HB	2.01	0.41
2:D:311:THR:HG23	2:D:328:THR:HG23	2.02	0.41
2:D:220:GLU:OE2	2:D:286:GLN:NE2	2.54	0.41
2:B:20:THR:O	2:B:94:GLN:HA	2.20	0.41
2:D:442:GLU:CD	2:D:454:ARG:HH12	2.24	0.41
1:A:672:PRO:HG2	1:A:677:ILE:HD11	2.03	0.41
2:B:77:GLU:HG3	2:B:78:ASP:N	2.35	0.41
2:D:23:GLU:HA	2:D:24:PRO:HD3	1.76	0.41
2:D:385:ARG:HG3	2:D:434:VAL:HG13	2.03	0.41
2:B:264:ALA:HA	2:B:267:LEU:HD13	2.02	0.41
2:B:443:ARG:HG2	2:B:461:CYS:HB2	2.02	0.41
2:B:451:LYS:HE3	2:B:453:LYS:CB	2.47	0.41
2:D:143:GLN:CD	2:D:210:HIS:HD1	2.24	0.41
2:D:374:ALA:HB1	2:D:377:ALA:CB	2.50	0.41
1:A:510:THR:HG21	1:A:542:ILE:HG13	2.03	0.41
2:B:265:SER:CB	2:B:272:VAL:HG11	2.51	0.41
1:C:459:VAL:HG12	1:C:470:THR:HG22	2.03	0.41
2:D:200:VAL:HG21	2:D:242:THR:HG21	2.02	0.41
1:C:446:GLN:HG3	1:C:801:MET:HG3	2.02	0.41
2:B:328:THR:HG23	2:B:329:THR:HG23	2.03	0.40
1:C:449:PHE:CE2	1:C:485:GLY:HA2	2.56	0.40
2:B:71:PHE:CE2	2:B:420:SER:HB2	2.55	0.40
2:D:264:ALA:HA	2:D:267:LEU:HD13	2.03	0.40
2:B:28:LEU:O	2:B:33:ARG:NH2	2.55	0.40
2:B:50:LEU:HD23	2:B:50:LEU:HA	1.89	0.40
2:D:29:PRO:O	2:D:33:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HB3	1:A:581:VAL:HB	2.04	0.40
1:A:689:LEU:HB2	1:A:701:HIS:HB2	2.03	0.40
2:B:350:ARG:O	2:B:355:SER:OG	2.39	0.40
1:C:787:TRP:CD1	1:C:801:MET:HB3	2.57	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:C:654:ARG:NH1	2:D:57:ASP:O[1_655]	2.12	0.08

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	353/388 (91%)	342 (97%)	10 (3%)	1 (0%)	41	64
1	C	353/388 (91%)	343 (97%)	10 (3%)	0	100	100
2	B	450/499 (90%)	429 (95%)	20 (4%)	1 (0%)	47	71
2	D	447/499 (90%)	426 (95%)	18 (4%)	3 (1%)	22	44
All	All	1603/1774 (90%)	1540 (96%)	58 (4%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	633	ASN
2	B	141	PRO
2	D	59	GLY
2	D	141	PRO
2	D	379	THR

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	301/328 (92%)	301 (100%)	0	100	100
1	C	301/328 (92%)	301 (100%)	0	100	100
2	B	381/411 (93%)	377 (99%)	4 (1%)	76	90
2	D	378/411 (92%)	370 (98%)	8 (2%)	53	78
All	All	1361/1478 (92%)	1349 (99%)	12 (1%)	78	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	47	SER
2	B	139	VAL
2	B	308	ARG
2	B	310	ARG
2	D	44	TYR
2	D	88	GLU
2	D	94	GLN
2	D	139	VAL
2	D	144	GLU
2	D	189	ASP
2	D	308	ARG
2	D	373	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	EDO	C	902	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	A	901	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	903	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	904	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	906	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	D	503	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	902	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	C	901	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	A	905	-	3,3,3	0.47	0	2,2,2	0.27	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	902	-	-	0/1/1/1	-
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	A	901	-	-	1/1/1/1	-
3	EDO	A	903	-	-	1/1/1/1	-
3	EDO	A	904	-	-	0/1/1/1	-
3	EDO	A	906	-	-	0/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	A	902	-	-	0/1/1/1	-
3	EDO	C	901	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	A	905	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	EDO	O1-C1-C2-O2
3	A	901	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	EDO	1	0
3	A	906	EDO	1	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	357/388 (92%)	0.13	7 (1%)	65	65	27, 39, 60, 94	0
1	C	357/388 (92%)	0.11	7 (1%)	65	65	27, 38, 63, 93	0
2	B	460/499 (92%)	0.55	39 (8%)	10	8	35, 58, 86, 99	0
2	D	457/499 (91%)	0.68	51 (11%)	5	4	32, 57, 88, 105	0
All	All	1631/1774 (91%)	0.40	104 (6%)	19	17	27, 47, 83, 105	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	139	VAL	6.2
2	D	374	ALA	5.7
2	D	375	SER	5.7
2	D	378	THR	5.2
2	D	137	ALA	5.1
2	B	431	LEU	4.7
2	D	210	HIS	4.7
2	B	160	ALA	4.5
2	B	272	VAL	4.4
2	B	271	HIS	4.4
2	D	33	ARG	4.4
2	D	431	LEU	4.2
2	B	379	THR	4.2
2	B	139	VAL	4.1
2	D	160	ALA	4.1
2	B	430	SER	4.1
2	D	430	SER	4.1
2	D	379	THR	4.0
2	B	137	ALA	3.9
2	D	138	ALA	3.7
2	D	429	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	57	ASP	3.7
2	D	208	SER	3.6
2	D	271	HIS	3.6
2	B	132	ALA	3.6
2	D	60	SER	3.6
1	C	434	SER	3.6
2	B	138	ALA	3.5
2	D	428	GLU	3.5
2	B	375	SER	3.5
1	A	753	GLN	3.4
2	D	214	GLU	3.4
2	D	27	GLU	3.4
2	B	85	LEU	3.3
2	D	373	ARG	3.3
2	B	429	GLY	3.3
2	B	424	ALA	3.1
2	D	54	SER	3.1
2	D	451	LYS	3.1
2	B	452	LYS	3.1
2	B	428	GLU	3.1
2	B	355	SER	3.1
2	D	376	SER	3.1
2	D	377	ALA	3.1
2	B	451	LYS	3.0
1	A	434	SER	3.0
1	C	753	GLN	2.9
2	D	32	LYS	2.9
2	D	55	MET	2.9
1	A	630	ARG	2.8
1	C	633	ASN	2.8
2	D	381	VAL	2.8
2	D	44	TYR	2.8
2	B	374	ALA	2.8
2	B	450	GLY	2.8
2	D	58	THR	2.7
2	D	23	GLU	2.7
2	D	161	SER	2.7
2	B	381	VAL	2.7
2	D	213	GLY	2.6
2	D	29	PRO	2.6
2	D	380	SER	2.6
1	C	432	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	425	THR	2.6
1	A	564	GLU	2.6
2	B	84	GLY	2.5
2	B	86	SER	2.5
2	B	141	PRO	2.5
2	D	402	TYR	2.5
2	B	258	SER	2.4
2	D	424	ALA	2.4
2	D	272	VAL	2.4
1	C	630	ARG	2.3
1	A	432	LEU	2.3
2	D	85	LEU	2.3
2	D	448	SER	2.3
2	B	161	SER	2.3
1	A	633	ASN	2.3
2	B	447	ALA	2.3
2	D	105	GLU	2.3
2	D	59	GLY	2.2
2	B	376	SER	2.2
2	B	11	PRO	2.2
2	B	210	HIS	2.2
2	B	380	SER	2.2
2	D	452	LYS	2.2
1	C	564	GLU	2.2
2	D	30	GLU	2.2
1	A	460	ALA	2.2
2	B	68	ASN	2.2
2	D	82	SER	2.2
2	B	378	THR	2.1
1	C	433	PRO	2.1
2	B	82	SER	2.1
2	B	128	ARG	2.1
2	D	206	THR	2.1
2	B	269	GLY	2.1
2	D	423	PRO	2.0
2	D	10	ALA	2.0
2	D	43	ARG	2.0
2	D	326	ASP	2.0
2	B	377	ALA	2.0
2	B	27	GLU	2.0
2	B	35	LEU	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	A	904	4/4	0.72	0.25	54,55,55,56	0
3	EDO	A	905	4/4	0.75	0.24	56,56,56,56	0
4	MG	A	907	1/1	0.80	0.32	45,45,45,45	0
3	EDO	A	902	4/4	0.81	0.37	44,44,44,45	0
3	EDO	A	903	4/4	0.82	0.34	40,41,43,44	0
3	EDO	D	503	4/4	0.84	0.24	53,53,54,55	0
3	EDO	C	902	4/4	0.87	0.25	47,49,52,52	0
3	EDO	A	906	4/4	0.88	0.20	51,52,53,53	0
3	EDO	D	502	4/4	0.88	0.19	48,49,49,49	0
3	EDO	A	901	4/4	0.89	0.22	41,43,44,44	0
3	EDO	C	901	4/4	0.90	0.12	46,47,48,48	0
3	EDO	D	501	4/4	0.92	0.28	27,28,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.