Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 01:33 pm BST

PDB ID	:	7ZAU
Title	:	Fascin-1 in complex with Nb 3E11
Authors	:	Burgess, S.G.; Bayliss, R.
Deposited on	:	2022-03-22
Resolution	:	2.20 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 (1)) were used in the production of this report:

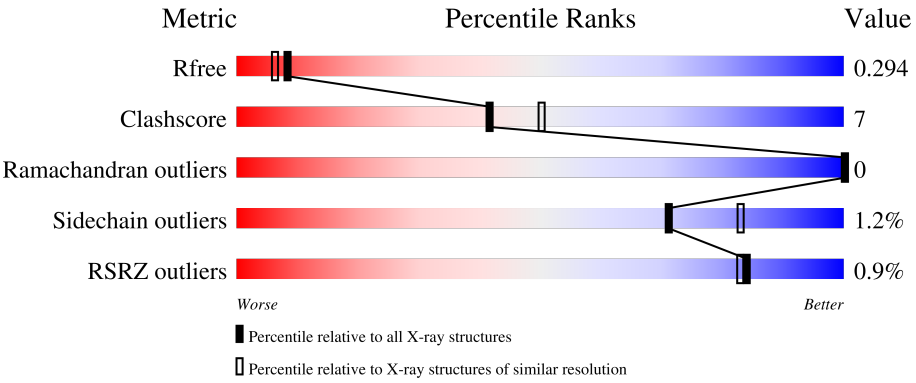
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	498	84% 13% •
1	C	498	% 78% 19% •
1	E	498	% 79% 17% •
1	G	498	% 83% 13% • •
2	B	132	2% 82% 13% • 5%

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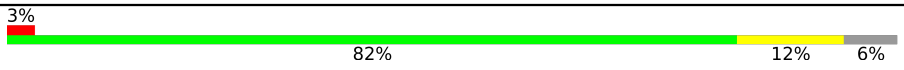
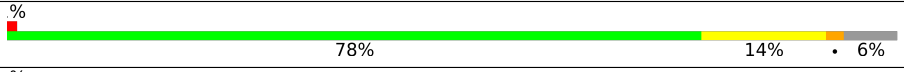
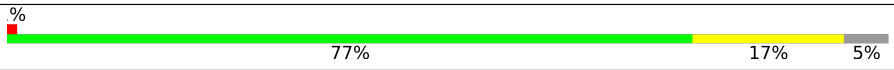
Mol	Chain	Length	Quality of chain
2	D	132	
2	F	132	
2	H	132	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19344 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 Fascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	1	0
			3697	2312	651	720	14			
1	C	480	Total	C	N	O	S	0	1	0
			3594	2248	627	705	14			
1	E	481	Total	C	N	O	S	0	0	0
			3624	2264	632	714	14			
1	G	480	Total	C	N	O	S	0	0	0
			3598	2252	626	706	14			

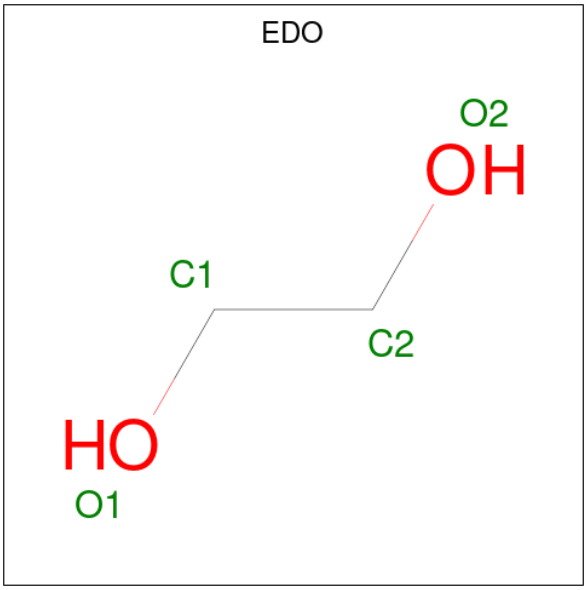
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q16658
A	-3	GLY	-	expression tag	UNP Q16658
A	-2	SER	-	expression tag	UNP Q16658
A	-1	GLU	-	expression tag	UNP Q16658
A	0	PHE	-	expression tag	UNP Q16658
C	-4	GLY	-	expression tag	UNP Q16658
C	-3	GLY	-	expression tag	UNP Q16658
C	-2	SER	-	expression tag	UNP Q16658
C	-1	GLU	-	expression tag	UNP Q16658
C	0	PHE	-	expression tag	UNP Q16658
E	-4	GLY	-	expression tag	UNP Q16658
E	-3	GLY	-	expression tag	UNP Q16658
E	-2	SER	-	expression tag	UNP Q16658
E	-1	GLU	-	expression tag	UNP Q16658
E	0	PHE	-	expression tag	UNP Q16658
G	-4	GLY	-	expression tag	UNP Q16658
G	-3	GLY	-	expression tag	UNP Q16658
G	-2	SER	-	expression tag	UNP Q16658
G	-1	GLU	-	expression tag	UNP Q16658
G	0	PHE	-	expression tag	UNP Q16658

- Molecule 2 is a protein called Nanobody 3E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			960	608	164	183	5			
2	D	124	Total	C	N	O	S	0	0	0
			943	598	159	181	5			
2	F	124	Total	C	N	O	S	0	0	0
			931	591	156	179	5			
2	H	125	Total	C	N	O	S	0	0	0
			954	606	161	182	5			

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

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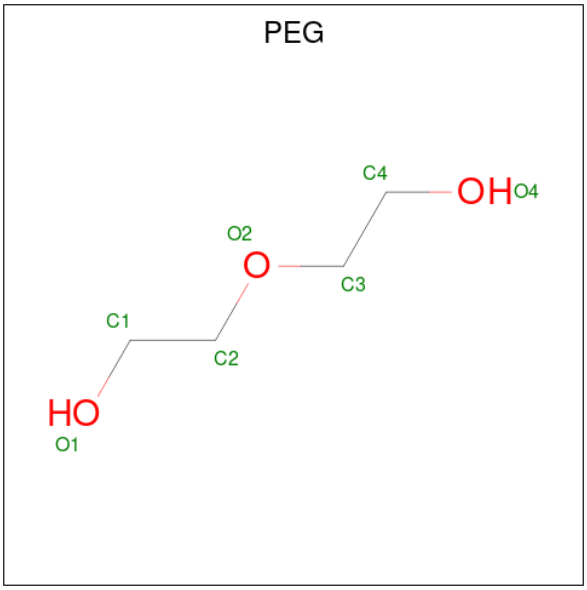
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	G	1	Total C O 7 4 3	0	0

- Molecule 5 is water.

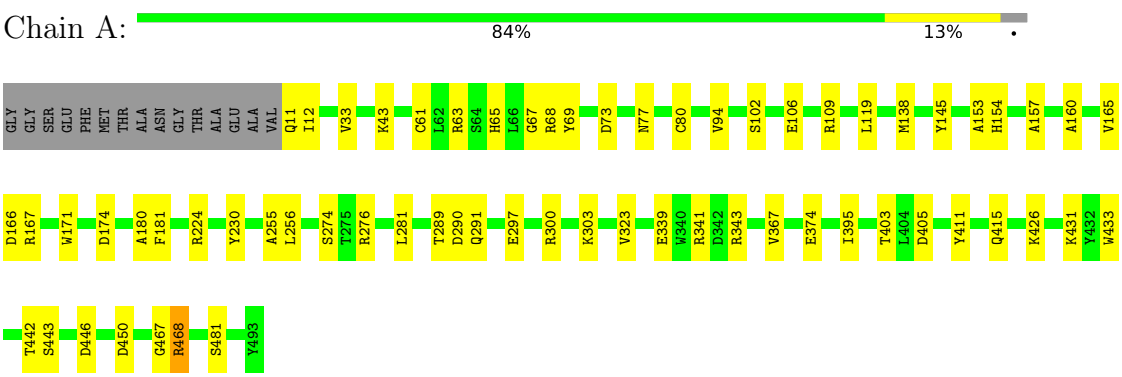
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	192	Total O 192 192	0	0
5	B	85	Total O 85 85	0	0
5	C	152	Total O 152 152	0	0
5	D	44	Total O 44 44	0	0
5	E	185	Total O 185 185	0	0
5	F	57	Total O 57 57	0	0
5	G	177	Total O 177 177	0	0
5	H	52	Total O 52 52	0	0

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.

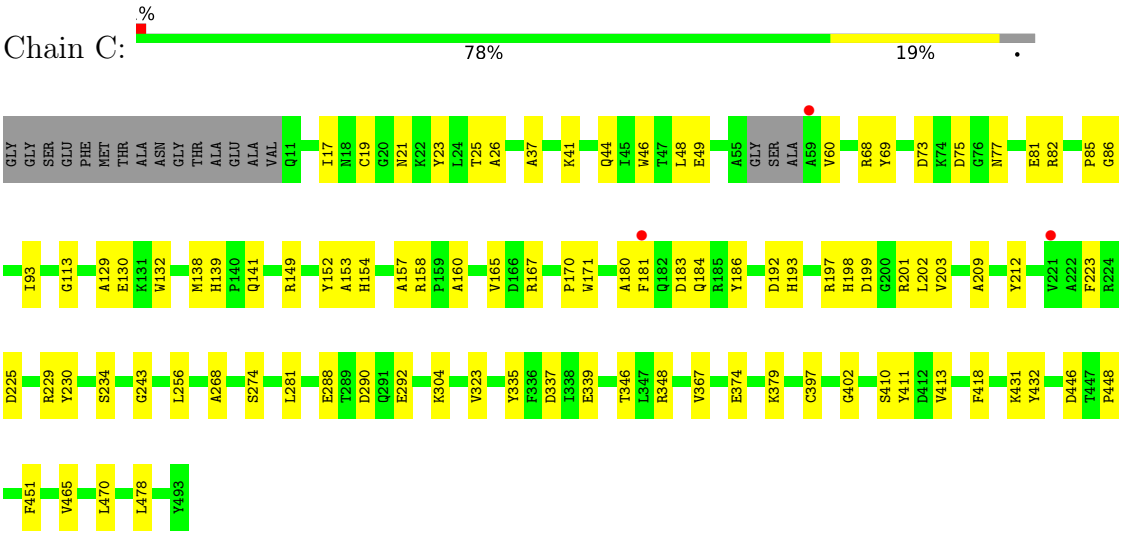
• Molecule 1: Fascin

Chain A:



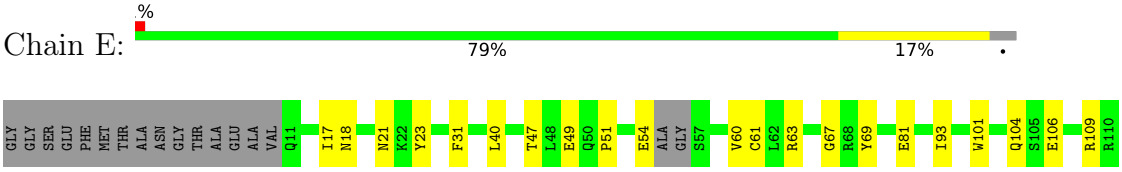
• Molecule 1: Fascin

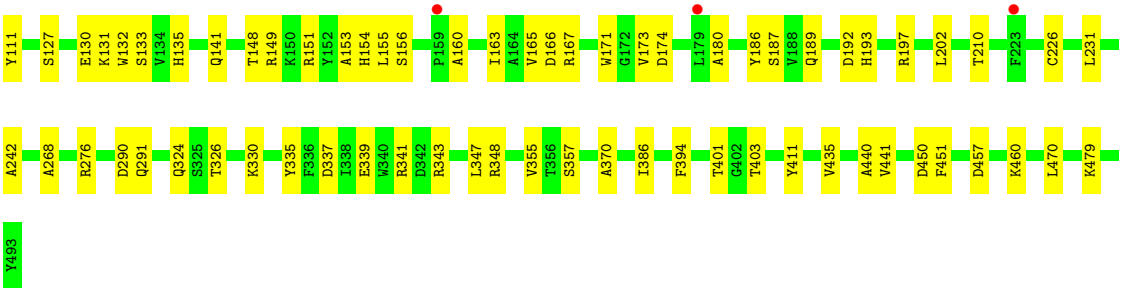
Chain C:



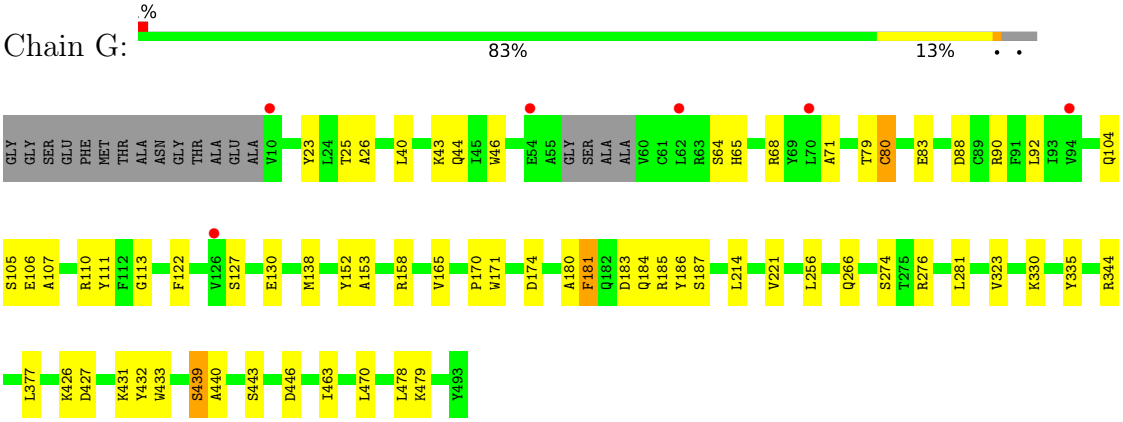
• Molecule 1: Fascin

Chain E:

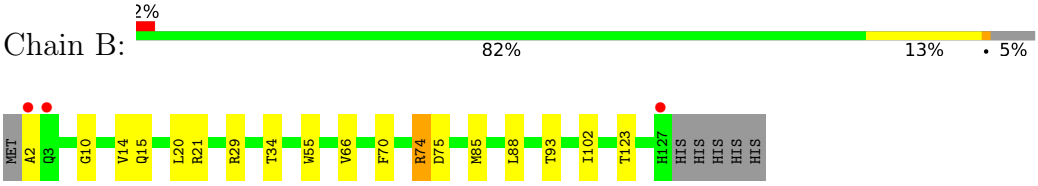




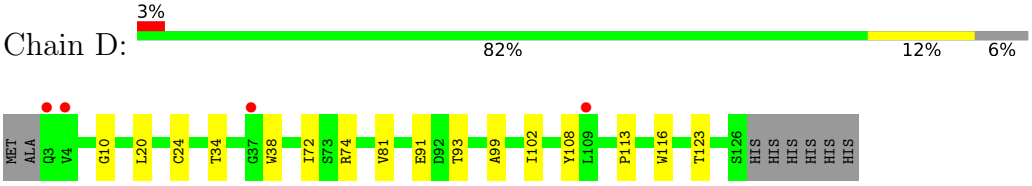
• Molecule 1: Fascin



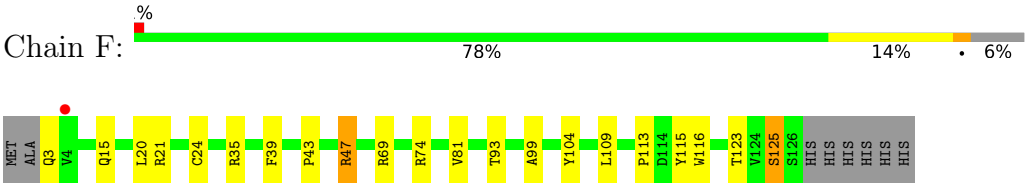
• Molecule 2: Nanobody 3E11



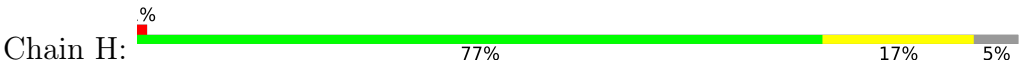
• Molecule 2: Nanobody 3E11

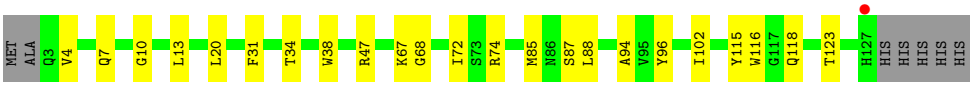


• Molecule 2: Nanobody 3E11



• Molecule 2: Nanobody 3E11




MET
ALA
Q3
V4
Q7
G10
L13
L20
F31
T34
W38
R47
K67
G68
I72
S73
R74
M85
N86
S87
L88
A94
V95
Y96
I102
Y115
W116
G117
Q118
T123
H127
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.91Å 210.32Å 105.47Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	59.44 – 2.20 105.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (59.44-2.20) 91.1 (105.16-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19_4085	Depositor
R, R_{free}	0.247 , 0.290 0.251 , 0.294	Depositor DCC
R_{free} test set	7700 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19344	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.37 % 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 3.2074e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, PEG

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	0.28	0/3777	0.49	0/5122
1	C	0.29	0/3672	0.50	0/4994
1	E	0.27	0/3702	0.49	0/5031
1	G	0.28	0/3675	0.50	0/4998
2	B	0.29	0/982	0.49	0/1331
2	D	0.28	0/965	0.48	0/1310
2	F	0.28	0/953	0.49	0/1295
2	H	0.30	0/976	0.50	0/1323
All	All	0.28	0/18702	0.50	0/25404

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	3697	0	3478	39	0
1	C	3594	0	3282	60	0
1	E	3624	0	3344	52	0
1	G	3598	0	3305	47	0
2	B	960	0	909	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	943	0	883	9	0
2	F	931	0	866	16	0
2	H	954	0	909	15	0
3	A	20	0	30	3	0
3	B	4	0	6	1	0
3	C	8	0	12	1	0
3	E	20	0	30	5	0
3	G	8	0	12	1	0
3	H	4	0	6	2	0
4	C	7	0	10	1	0
4	E	21	0	30	0	0
4	G	7	0	10	1	0
5	A	192	0	0	3	0
5	B	85	0	0	1	0
5	C	152	0	0	3	0
5	D	44	0	0	0	0
5	E	185	0	0	5	0
5	F	57	0	0	5	0
5	G	177	0	0	0	0
5	H	52	0	0	0	0
All	All	19344	0	17122	248	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 7.

All (248) 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)
3:E:506:EDO:H21	5:E:697:HOH:O	1.48	1.13
1:C:68:ARG:HD2	1:C:81:GLU:HA	1.50	0.92
2:F:47:ARG:CD	5:F:247:HOH:O	2.22	0.87
1:E:187:SER:HA	5:E:604:HOH:O	1.74	0.86
1:G:71:ALA:HB3	1:G:79:THR:OG1	1.80	0.81
1:G:105:SER:HB3	1:G:110:ARG:H	1.49	0.77
1:A:106:GLU:O	1:A:109:ARG:NH1	2.21	0.74
2:F:43:PRO:HB3	5:F:252:HOH:O	1.87	0.73
1:C:48:LEU:HD11	1:C:60:VAL:HG13	1.70	0.72
2:H:7:GLN:HB2	2:H:118:GLN:HE22	1.56	0.71
4:C:503:PEG:H11	2:H:67:LYS:HG2	1.74	0.69
1:G:106:GLU:HG2	1:G:107:ALA:H	1.57	0.69
2:F:35:ARG:NH2	2:F:109:LEU:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ASP:HA	3:B:201:EDO:H21	1.74	0.67
1:E:151:ARG:HH12	3:E:504:EDO:H12	1.59	0.67
1:C:268:ALA:HA	3:C:501:EDO:H12	1.76	0.67
2:F:47:ARG:CG	5:F:247:HOH:O	2.41	0.67
1:A:415:GLN:HB2	1:A:426:LYS:HG2	1.77	0.66
1:G:106:GLU:OE1	1:G:106:GLU:N	2.25	0.66
2:F:47:ARG:HG3	5:F:247:HOH:O	1.96	0.65
2:B:2:ALA:HB1	2:B:29:ARG:HB2	1.79	0.65
1:G:88:ASP:HA	1:G:106:GLU:HG3	1.77	0.65
2:D:91:GLU:OE1	2:D:91:GLU:N	2.30	0.64
1:E:163:ILE:HG13	1:E:202:LEU:HD11	1.79	0.64
1:A:290:ASP:H	3:A:502:EDO:H22	1.62	0.64
2:B:21:ARG:NH1	5:B:303:HOH:O	2.33	0.62
1:C:154:HIS:CD2	1:C:167:ARG:HG3	2.35	0.62
1:E:106:GLU:HA	1:E:109:ARG:HH12	1.66	0.61
1:C:68:ARG:HD2	1:C:81:GLU:CA	2.28	0.61
2:H:47:ARG:HD3	2:H:116:TRP:CH2	2.36	0.61
1:G:68:ARG:HB3	1:G:80:CYS:O	2.01	0.60
3:E:506:EDO:C2	5:E:697:HOH:O	2.24	0.60
1:C:21:ASN:ND2	5:C:601:HOH:O	2.29	0.60
1:C:139:HIS:HE1	1:C:141:GLN:HG3	1.67	0.60
1:G:138:MET:HE1	1:G:256:LEU:HB3	1.83	0.60
1:G:180:ALA:HB1	3:G:501:EDO:H21	1.83	0.60
1:E:17:ILE:HG23	1:E:21:ASN:HA	1.85	0.58
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.84	0.58
1:E:435:VAL:HG12	1:E:441:VAL:HG22	1.86	0.58
1:A:43:LYS:HA	1:A:65:HIS:CD2	2.39	0.58
1:A:181:PHE:H	3:A:503:EDO:H21	1.68	0.57
1:C:149:ARG:NH1	5:C:606:HOH:O	2.37	0.57
1:G:64:SER:OG	1:G:65:HIS:N	2.38	0.57
1:G:64:SER:HB3	1:G:68:ARG:H	1.68	0.57
1:C:139:HIS:CE1	1:C:141:GLN:HG3	2.40	0.56
1:G:23:TYR:CE2	1:G:40:LEU:HB2	2.39	0.56
1:A:154:HIS:CD2	1:A:167:ARG:HG3	2.40	0.56
1:C:183:ASP:OD1	1:C:184:GLN:N	2.38	0.56
1:C:181:PHE:CZ	1:C:410:SER:HB3	2.41	0.56
1:G:183:ASP:OD1	1:G:184:GLN:N	2.39	0.56
1:E:173:VAL:HG21	3:E:506:EDO:H12	1.87	0.56
2:F:47:ARG:HD3	5:F:247:HOH:O	1.96	0.56
2:H:68:GLY:H	3:H:201:EDO:H12	1.71	0.56
1:A:94:VAL:HB	1:A:102:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:O	1:A:303:LYS:NZ	2.30	0.56
1:E:60:VAL:HG21	1:E:93:ILE:HD12	1.88	0.56
1:C:153:ALA:HA	1:C:165:VAL:HA	1.87	0.55
2:D:34:THR:HG22	2:D:102:ILE:O	2.04	0.55
1:A:339:GLU:OE1	1:A:341:ARG:NH2	2.33	0.55
1:E:63:ARG:NE	1:E:67:GLY:HA2	2.22	0.55
1:G:92:LEU:HB2	1:G:104:GLN:HB3	1.89	0.55
1:E:104:GLN:OE1	1:E:109:ARG:NH1	2.40	0.55
1:A:431:LYS:NZ	1:A:446:ASP:OD1	2.34	0.54
1:E:268:ALA:HA	3:E:505:EDO:H12	1.88	0.54
2:D:93:THR:HG23	2:D:123:THR:HA	1.90	0.54
1:A:157:ALA:HA	1:A:160:ALA:HA	1.90	0.54
1:C:230:TYR:O	1:C:243:GLY:N	2.32	0.54
1:E:347:LEU:HB2	1:E:355:VAL:HG22	1.88	0.54
2:H:34:THR:HG22	2:H:102:ILE:O	2.07	0.54
1:A:224:ARG:NH1	5:A:605:HOH:O	2.41	0.54
1:G:113:GLY:HA3	1:G:130:GLU:HG3	1.90	0.53
1:G:26:ALA:HB2	1:G:46:TRP:CZ2	2.43	0.53
1:A:138:MET:HE1	1:A:256:LEU:HB3	1.91	0.52
2:B:85:MET:HB3	2:B:88:LEU:HD21	1.91	0.52
1:E:31:PHE:CG	1:E:81:GLU:HG3	2.44	0.52
2:F:93:THR:HG23	2:F:123:THR:HA	1.92	0.52
1:G:153:ALA:HA	1:G:165:VAL:HA	1.91	0.52
1:C:274:SER:HB2	1:C:292:GLU:HG3	1.91	0.52
2:H:38:TRP:HD1	2:H:72:ILE:HD12	1.74	0.52
1:A:281:LEU:HD12	1:A:323:VAL:HG12	1.92	0.52
1:G:431:LYS:NZ	1:G:446:ASP:OD1	2.43	0.52
1:A:224:ARG:NH2	5:A:606:HOH:O	2.42	0.51
1:E:324:GLN:HB3	1:E:326:THR:HG23	1.91	0.51
1:C:19:CYS:HB3	1:C:129:ALA:HA	1.92	0.51
1:G:183:ASP:OD1	1:G:185:ARG:HG2	2.10	0.51
1:E:23:TYR:CE2	1:E:40:LEU:HB2	2.45	0.51
1:E:343:ARG:NH1	5:E:607:HOH:O	2.42	0.51
2:H:10:GLY:O	2:H:20:LEU:HD11	2.11	0.51
1:C:167:ARG:NH2	1:C:290:ASP:OD2	2.42	0.51
1:C:281:LEU:HD12	1:C:323:VAL:HG12	1.92	0.51
1:C:470:LEU:HD23	1:C:478:LEU:HD21	1.92	0.51
1:E:192:ASP:O	1:E:193:HIS:HB2	2.11	0.51
1:G:71:ALA:HB3	1:G:79:THR:HG1	1.75	0.51
1:G:80:CYS:O	1:G:80:CYS:SG	2.68	0.51
1:A:73:ASP:HB2	1:A:77:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:HG22	2:B:102:ILE:O	2.11	0.50
1:A:224:ARG:HB3	1:A:230:TYR:CE1	2.47	0.49
1:G:439:SER:O	1:G:439:SER:OG	2.30	0.49
1:E:401:THR:HG22	1:E:403:THR:HG23	1.94	0.49
2:B:10:GLY:O	2:B:20:LEU:HD21	2.12	0.49
2:B:93:THR:HG23	2:B:123:THR:HA	1.94	0.49
1:E:51:PRO:HB2	1:E:54:GLU:HB2	1.95	0.49
1:G:106:GLU:HG2	1:G:107:ALA:N	2.27	0.49
1:E:226:CYS:SG	5:E:750:HOH:O	2.60	0.48
1:E:197:ARG:HA	1:E:210:THR:HG22	1.94	0.48
1:E:440:ALA:HA	1:E:479:LYS:HG2	1.95	0.48
1:G:183:ASP:CG	1:G:184:GLN:H	2.17	0.48
1:E:154:HIS:CD2	1:E:167:ARG:HG3	2.48	0.48
1:C:451:PHE:CD1	1:C:465:VAL:HB	2.48	0.48
2:D:99:ALA:HB1	2:D:113:PRO:HB3	1.94	0.48
1:E:101:TRP:O	1:E:131:LYS:HA	2.13	0.48
1:G:427:ASP:OD2	1:G:443:SER:OG	2.27	0.48
2:D:24:CYS:HB3	2:D:81:VAL:HG13	1.95	0.48
1:G:105:SER:HB3	1:G:110:ARG:N	2.23	0.48
1:G:127:SER:OG	1:G:130:GLU:OE1	2.30	0.48
2:H:87:SER:O	2:H:87:SER:OG	2.30	0.48
1:E:148:THR:HG23	1:E:149:ARG:HG2	1.95	0.48
1:E:167:ARG:NH2	1:E:290:ASP:OD2	2.47	0.48
1:A:224:ARG:HB3	1:A:230:TYR:CD1	2.49	0.47
1:C:26:ALA:HB2	1:C:46:TRP:CZ2	2.49	0.47
1:C:201:ARG:HG2	1:C:202:LEU:N	2.29	0.47
1:G:186:TYR:CD1	1:G:214:LEU:HD13	2.48	0.47
1:C:225:ASP:OD1	1:C:229:ARG:N	2.48	0.47
1:G:25:THR:HG23	1:G:44:GLN:HG3	1.95	0.47
1:E:40:LEU:HD22	1:E:135:HIS:HD2	1.79	0.47
1:E:104:GLN:HB2	1:E:111:TYR:CE1	2.49	0.47
1:G:180:ALA:HB3	1:G:187:SER:OG	2.14	0.47
1:G:221:VAL:HG11	1:G:256:LEU:HG	1.96	0.47
2:F:20:LEU:HD23	2:F:21:ARG:N	2.30	0.47
1:E:47:THR:HG22	1:E:49:GLU:HG3	1.96	0.47
1:E:141:GLN:HE22	1:E:386:ILE:HA	1.80	0.47
1:G:90:ARG:O	1:G:106:GLU:HB3	2.15	0.47
1:C:73:ASP:HB3	1:C:75:ASP:H	1.80	0.47
1:G:105:SER:N	1:G:110:ARG:O	2.46	0.47
2:H:31:PHE:HB2	2:H:34:THR:HG23	1.97	0.47
1:C:69:TYR:CZ	1:C:85:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:GLN:HE21	1:E:193:HIS:HA	1.80	0.46
1:E:347:LEU:HB2	1:E:355:VAL:CG2	2.44	0.46
1:A:289:THR:HB	3:A:502:EDO:H21	1.97	0.46
1:A:291:GLN:HE22	2:F:69:ARG:HD3	1.79	0.46
1:A:11:GLN:HG2	1:A:12:ILE:H	1.80	0.46
2:B:55:TRP:CE3	2:B:74:ARG:HD3	2.50	0.46
1:E:339:GLU:CD	1:E:341:ARG:HE	2.18	0.46
1:G:266:GLN:HB3	1:G:377:LEU:HB3	1.97	0.46
1:E:156:SER:HB3	1:E:160:ALA:HB1	1.98	0.46
1:E:341:ARG:NH2	1:E:370:ALA:HB3	2.31	0.46
2:F:113:PRO:HG2	2:F:116:TRP:CZ2	2.50	0.46
1:G:330:LYS:HD2	1:G:335:TYR:OH	2.15	0.46
1:C:431:LYS:NZ	1:C:446:ASP:OD1	2.42	0.45
1:C:181:PHE:HZ	1:C:410:SER:HB3	1.79	0.45
1:C:48:LEU:HD11	1:C:60:VAL:CG1	2.44	0.45
1:A:367:VAL:HG21	1:A:374:GLU:OE2	2.15	0.45
1:C:367:VAL:HG21	1:C:374:GLU:OE2	2.15	0.45
1:G:440:ALA:HA	1:G:479:LYS:HG2	1.98	0.45
1:G:433:TRP:CD1	1:G:443:SER:HB2	2.52	0.45
1:G:274:SER:OG	1:G:276:ARG:HG3	2.17	0.45
1:E:394:PHE:CG	1:E:411:TYR:HB3	2.51	0.45
1:C:192:ASP:O	1:C:193:HIS:HB2	2.17	0.45
1:G:111:TYR:HB3	1:G:130:GLU:HG2	1.99	0.45
1:A:274:SER:OG	1:A:276:ARG:HG3	2.17	0.45
1:C:397:CYS:SG	1:C:402:GLY:HA2	2.57	0.45
1:G:158:ARG:HE	1:G:158:ARG:HB2	1.53	0.45
1:A:153:ALA:HA	1:A:165:VAL:HA	1.99	0.44
1:E:337:ASP:HB2	1:E:348:ARG:HB3	1.99	0.44
1:C:60:VAL:HG11	1:C:93:ILE:HD11	1.99	0.44
1:C:152:TYR:CE2	1:C:170:PRO:HD3	2.51	0.44
1:E:231:LEU:HA	1:E:242:ALA:HA	1.99	0.44
1:A:395:ILE:HA	1:A:405:ASP:O	2.17	0.44
1:G:426:LYS:HB3	1:G:432:TYR:CD1	2.52	0.44
1:A:61:CYS:HB3	1:A:69:TYR:HD2	1.83	0.44
1:G:470:LEU:HD23	1:G:478:LEU:HD21	2.00	0.44
2:H:94:ALA:HB3	2:H:96:TYR:CE1	2.53	0.44
1:C:411:TYR:HE1	1:C:413:VAL:HG22	1.81	0.43
1:A:174:ASP:OD1	1:A:174:ASP:N	2.49	0.43
1:C:167:ARG:HH22	1:C:290:ASP:CG	2.20	0.43
1:C:197:ARG:HE	1:C:199:ASP:CG	2.22	0.43
2:D:113:PRO:HG2	2:D:116:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:VAL:HG22	2:H:115:TYR:CD2	2.53	0.43
1:A:467:GLY:O	1:A:468:ARG:NH1	2.51	0.43
1:C:25:THR:HG23	1:C:44:GLN:HG3	1.99	0.43
1:E:155:LEU:HD13	2:F:104:TYR:CG	2.54	0.43
2:D:10:GLY:O	2:D:20:LEU:HD11	2.19	0.43
1:C:23:TYR:HB2	1:C:37:ALA:HB3	2.00	0.43
1:E:341:ARG:HH22	1:E:370:ALA:HB3	1.83	0.43
2:F:24:CYS:HB3	2:F:81:VAL:HG13	1.99	0.43
1:G:463:ILE:HG22	1:G:470:LEU:HD13	2.01	0.43
1:C:180:ALA:O	1:C:186:TYR:HA	2.18	0.43
1:A:433:TRP:CD1	1:A:443:SER:HB2	2.54	0.43
1:E:174:ASP:OD1	1:E:174:ASP:N	2.52	0.43
1:A:343:ARG:NH2	1:A:450:ASP:OD2	2.37	0.43
1:C:158:ARG:N	1:C:160:ALA:HB2	2.33	0.43
1:E:127:SER:HB3	1:E:130:GLU:OE1	2.19	0.43
1:G:152:TYR:CE2	1:G:170:PRO:HD3	2.54	0.43
1:E:343:ARG:NH2	1:E:450:ASP:OD2	2.46	0.43
1:A:33:VAL:HG23	1:A:119:LEU:HD12	2.00	0.43
1:C:86:GLY:HA3	5:C:718:HOH:O	2.19	0.43
2:F:39:PHE:HE1	2:F:99:ALA:HB3	1.85	0.42
1:C:304:LYS:HB3	1:C:335:TYR:HB3	2.01	0.42
1:C:339:GLU:HB3	1:C:346:THR:OG1	2.20	0.42
1:E:451:PHE:HE2	1:E:470:LEU:HD11	1.84	0.42
4:G:503:PEG:H41	4:G:503:PEG:H21	1.76	0.42
1:C:68:ARG:HD2	1:C:82:ARG:N	2.33	0.42
1:A:154:HIS:NE2	1:A:166:ASP:OD1	2.36	0.42
1:C:138:MET:HE3	1:C:256:LEU:HB3	2.02	0.42
1:C:379:LYS:HD3	1:C:418:PHE:CD2	2.55	0.42
1:E:18:ASN:HB3	1:E:132:TRP:CZ3	2.55	0.42
1:C:113:GLY:HA3	1:C:130:GLU:HG3	2.01	0.42
2:F:99:ALA:HB1	2:F:113:PRO:HB3	2.02	0.42
1:A:403:THR:HA	1:A:442:THR:HG22	2.02	0.42
2:F:15:GLN:HA	2:F:125:SER:OG	2.20	0.42
1:C:197:ARG:NH1	1:C:203:VAL:HG11	2.35	0.41
2:H:68:GLY:H	3:H:201:EDO:C1	2.33	0.41
1:A:297:GLU:OE2	5:A:601:HOH:O	2.22	0.41
2:B:66:VAL:HG13	2:B:70:PHE:HB2	2.02	0.41
1:E:276:ARG:HG2	1:E:291:GLN:OE1	2.20	0.41
2:H:47:ARG:HD3	2:H:116:TRP:CZ3	2.55	0.41
1:A:180:ALA:HB2	1:A:411:TYR:OH	2.19	0.41
1:C:93:ILE:N	1:C:93:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HB2	1:A:80:CYS:SG	2.60	0.41
1:C:68:ARG:HD2	1:C:82:ARG:H	1.85	0.41
1:C:337:ASP:HB2	1:C:348:ARG:HB3	2.01	0.41
1:C:432:TYR:CZ	1:C:448:PRO:HG3	2.56	0.41
1:G:344:ARG:NH1	1:G:377:LEU:HD13	2.36	0.41
1:A:145:TYR:HB3	1:A:255:ALA:HB3	2.02	0.41
1:C:17:ILE:O	1:C:132:TRP:HA	2.21	0.41
1:E:457:ASP:HB3	1:E:460:LYS:HB2	2.02	0.41
1:C:49:GLU:OE2	1:C:69:TYR:OH	2.37	0.41
1:E:330:LYS:HD3	1:E:335:TYR:OH	2.21	0.41
1:A:109:ARG:HD2	1:A:109:ARG:N	2.36	0.41
2:B:14:VAL:HG12	2:B:15:GLN:O	2.20	0.41
1:E:154:HIS:NE2	1:E:166:ASP:OD1	2.42	0.41
2:F:3:GLN:HA	2:F:115:TYR:CZ	2.55	0.41
1:G:281:LEU:HD12	1:G:323:VAL:HG12	2.03	0.41
1:A:63:ARG:HD2	1:A:67:GLY:HA2	2.03	0.41
1:C:198:HIS:ND1	1:C:209:ALA:HB1	2.36	0.41
2:H:13:LEU:HD22	2:H:123:THR:HB	2.03	0.41
1:C:73:ASP:OD2	1:C:77:ASN:HB2	2.22	0.40
1:C:223:PHE:O	1:C:230:TYR:HA	2.21	0.40
1:C:212:TYR:CD2	1:C:225:ASP:HA	2.56	0.40
1:E:61:CYS:HB3	1:E:69:TYR:HD2	1.85	0.40
1:G:174:ASP:OD1	1:G:174:ASP:N	2.54	0.40
1:C:201:ARG:HG2	1:C:202:LEU:H	1.86	0.40
2:D:38:TRP:HD1	2:D:72:ILE:HD12	1.86	0.40
1:C:288:GLU:N	2:D:108:TYR:OH	2.42	0.40
1:E:180:ALA:O	1:E:186:TYR:HA	2.21	0.40
1:G:181:PHE:CD1	1:G:181:PHE:N	2.90	0.40
1:C:157:ALA:C	1:C:160:ALA:HB2	2.41	0.40
1:E:153:ALA:HA	1:E:165:VAL:HA	2.04	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	482/498 (97%)	457 (95%)	25 (5%)	0	100	100
1	C	477/498 (96%)	434 (91%)	43 (9%)	0	100	100
1	E	477/498 (96%)	447 (94%)	30 (6%)	0	100	100
1	G	476/498 (96%)	440 (92%)	36 (8%)	0	100	100
2	B	124/132 (94%)	120 (97%)	4 (3%)	0	100	100
2	D	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
2	F	122/132 (92%)	118 (97%)	4 (3%)	0	100	100
2	H	123/132 (93%)	121 (98%)	2 (2%)	0	100	100
All	All	2403/2520 (95%)	2256 (94%)	147 (6%)	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	376/407 (92%)	373 (99%)	3 (1%)	81	90
1	C	351/407 (86%)	348 (99%)	3 (1%)	78	88
1	E	362/407 (89%)	359 (99%)	3 (1%)	81	90
1	G	355/407 (87%)	348 (98%)	7 (2%)	55	69
2	B	97/108 (90%)	96 (99%)	1 (1%)	76	86
2	D	95/108 (88%)	94 (99%)	1 (1%)	73	85
2	F	93/108 (86%)	90 (97%)	3 (3%)	39	50
2	H	98/108 (91%)	97 (99%)	1 (1%)	76	86
All	All	1827/2060 (89%)	1805 (99%)	22 (1%)	71	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	TRP
1	A	468	ARG
1	A	481	SER
2	B	74	ARG
1	C	41	LYS
1	C	171	TRP
1	C	234	SER
2	D	74	ARG
1	E	133	SER
1	E	171	TRP
1	E	357	SER
2	F	47	ARG
2	F	74	ARG
2	F	125	SER
1	G	43	LYS
1	G	80	CYS
1	G	83	GLU
1	G	122	PHE
1	G	171	TRP
1	G	181	PHE
1	G	439	SER
2	H	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	118	GLN

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)

21 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	502	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	E	506	-	3,3,3	0.43	0	2,2,2	0.31	0
4	PEG	G	503	-	6,6,6	0.12	0	5,5,5	0.13	0
3	EDO	G	502	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	A	503	-	3,3,3	0.42	0	2,2,2	0.49	0
3	EDO	G	501	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	E	508	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.34	0
4	PEG	E	503	-	6,6,6	0.17	0	5,5,5	0.22	0
4	PEG	C	503	-	6,6,6	0.12	0	5,5,5	0.11	0
3	EDO	E	507	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	A	501	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	E	504	-	3,3,3	0.47	0	2,2,2	0.20	0
3	EDO	B	201	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	E	505	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	C	501	-	3,3,3	0.47	0	2,2,2	0.22	0
3	EDO	H	201	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.42	0
4	PEG	E	501	-	6,6,6	0.12	0	5,5,5	0.08	0
4	PEG	E	502	-	6,6,6	0.11	0	5,5,5	0.09	0
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.26	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	502	-	-	1/1/1/1	-
3	EDO	E	506	-	-	1/1/1/1	-
4	PEG	G	503	-	-	1/4/4/4	-
3	EDO	G	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	G	501	-	-	0/1/1/1	-
3	EDO	E	508	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
4	PEG	E	503	-	-	1/4/4/4	-
4	PEG	C	503	-	-	1/4/4/4	-
3	EDO	E	507	-	-	0/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-
3	EDO	E	504	-	-	0/1/1/1	-
3	EDO	B	201	-	-	1/1/1/1	-
3	EDO	E	505	-	-	0/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	H	201	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
4	PEG	E	501	-	-	0/4/4/4	-
4	PEG	E	502	-	-	0/4/4/4	-
3	EDO	A	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	EDO	O1-C1-C2-O2
3	E	506	EDO	O1-C1-C2-O2
4	C	503	PEG	C4-C3-O2-C2
4	G	503	PEG	C4-C3-O2-C2
3	C	502	EDO	O1-C1-C2-O2
3	E	508	EDO	O1-C1-C2-O2
4	E	503	PEG	C4-C3-O2-C2
3	A	502	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	506	EDO	3	0
4	G	503	PEG	1	0
3	A	503	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	EDO	1	0
4	C	503	PEG	1	0
3	E	504	EDO	1	0
3	B	201	EDO	1	0
3	E	505	EDO	1	0
3	C	501	EDO	1	0
3	H	201	EDO	2	0
3	A	502	EDO	2	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	483/498 (96%)	-0.27	0 100 100	37, 56, 79, 94	0
1	C	480/498 (96%)	-0.17	3 (0%) 89 88	39, 63, 97, 111	0
1	E	481/498 (96%)	-0.26	3 (0%) 89 88	34, 59, 86, 102	0
1	G	480/498 (96%)	-0.17	6 (1%) 77 75	38, 60, 95, 110	0
2	B	126/132 (95%)	-0.22	3 (2%) 59 56	38, 52, 72, 80	0
2	D	124/132 (93%)	0.07	4 (3%) 47 45	44, 65, 81, 91	0
2	F	124/132 (93%)	-0.17	1 (0%) 86 85	40, 58, 78, 90	0
2	H	125/132 (94%)	-0.26	1 (0%) 86 85	38, 53, 68, 88	0
All	All	2423/2520 (96%)	-0.20	21 (0%) 84 83	34, 59, 91, 111	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ALA	5.5
1	G	10	VAL	4.6
2	D	109	LEU	4.3
2	D	4	VAL	3.6
1	C	59	ALA	3.6
1	C	181	PHE	3.2
1	G	94	VAL	3.1
2	B	127	HIS	3.0
2	D	37	GLY	3.0
1	G	62	LEU	2.7
1	E	159	PRO	2.7
2	H	127	HIS	2.5
1	G	126	VAL	2.5
1	E	179	LEU	2.4
2	B	3	GLN	2.4
1	E	223	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	54	GLU	2.2
1	C	221	VAL	2.2
2	D	3	GLN	2.1
2	F	4	VAL	2.1
1	G	70	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	E	504	4/4	0.42	0.18	75,80,80,82	0
4	PEG	E	501	7/7	0.67	0.13	85,91,93,95	0
3	EDO	C	502	4/4	0.70	0.22	61,68,76,77	0
3	EDO	G	501	4/4	0.74	0.31	60,63,68,68	0
3	EDO	C	501	4/4	0.75	0.16	53,56,56,64	0
4	PEG	E	503	7/7	0.76	0.20	52,59,69,70	0
3	EDO	E	506	4/4	0.77	0.24	51,52,56,61	0
4	PEG	E	502	7/7	0.78	0.21	53,65,70,71	0
3	EDO	A	504	4/4	0.82	0.17	62,66,68,71	0
4	PEG	G	503	7/7	0.82	0.33	49,59,62,69	0
3	EDO	E	507	4/4	0.83	0.18	42,49,53,56	0
3	EDO	E	505	4/4	0.85	0.12	46,47,47,54	0
3	EDO	H	201	4/4	0.85	0.22	49,52,53,57	0
3	EDO	G	502	4/4	0.86	0.21	57,57,59,61	0
3	EDO	A	501	4/4	0.86	0.14	66,70,71,73	0
3	EDO	A	502	4/4	0.87	0.17	47,56,58,67	0
3	EDO	B	201	4/4	0.89	0.18	46,47,52,56	0
3	EDO	A	503	4/4	0.90	0.17	50,53,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	C	503	7/7	0.90	0.29	58,61,63,72	0
3	EDO	E	508	4/4	0.90	0.15	60,60,63,64	0
3	EDO	A	505	4/4	0.93	0.13	64,66,69,73	0

6.5 Other polymers (i)

There are no such residues in this entry.