Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 03:19 PM EDT

PDB ID	:	3DXB
Title	:	Structure of the UHM domain of Puf60 fused to thioredoxin
Authors	:	Corsini, L.; Hothorn, M.; Scheffzek, K.; Stier, G.; Sattler, M.
Deposited on	:	2008-07-24
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:

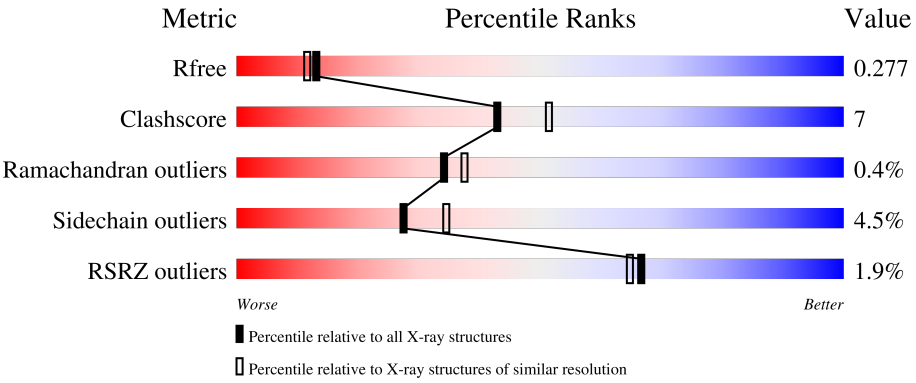
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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.



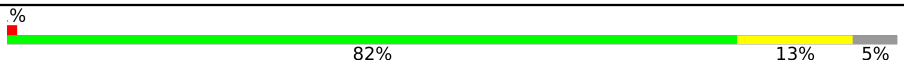
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	222	3% 85% 10%
1	B	222	3% 81% 11% 5%
1	C	222	% 81% 13% 5%
1	D	222	4% 81% 13%
1	E	222	3% 84% 9% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	222	
1	G	222	
1	H	222	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14337 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 thioredoxin N-terminally fused to Puf60(UHM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1655	1047	270	330	8			
1	B	211	Total	C	N	O	S	0	1	0
			1624	1030	267	320	7			
1	C	211	Total	C	N	O	S	0	4	0
			1657	1046	270	334	7			
1	D	216	Total	C	N	O	S	0	2	0
			1684	1064	276	336	8			
1	E	210	Total	C	N	O	S	0	0	0
			1622	1027	265	323	7			
1	F	211	Total	C	N	O	S	0	1	0
			1636	1035	267	327	7			
1	G	211	Total	C	N	O	S	0	0	0
			1630	1031	266	326	7			
1	H	211	Total	C	N	O	S	0	0	0
			1630	1031	266	326	7			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	MET	-	expression tag	UNP P0AA27
A	336	LYS	-	expression tag	UNP P0AA27
A	337	HIS	-	expression tag	UNP P0AA27
A	338	HIS	-	expression tag	UNP P0AA27
A	339	HIS	-	expression tag	UNP P0AA27
A	340	HIS	-	expression tag	UNP P0AA27
A	341	HIS	-	expression tag	UNP P0AA27
A	342	HIS	-	expression tag	UNP P0AA27
A	343	PRO	-	expression tag	UNP P0AA27
A	453	GLY	-	linker	UNP Q9UHX1
A	454	SER	-	linker	UNP Q9UHX1
A	455	ALA	-	linker	UNP Q9UHX1
A	456	MET	-	linker	UNP Q9UHX1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	335	MET	-	expression tag	UNP P0AA27
B	336	LYS	-	expression tag	UNP P0AA27
B	337	HIS	-	expression tag	UNP P0AA27
B	338	HIS	-	expression tag	UNP P0AA27
B	339	HIS	-	expression tag	UNP P0AA27
B	340	HIS	-	expression tag	UNP P0AA27
B	341	HIS	-	expression tag	UNP P0AA27
B	342	HIS	-	expression tag	UNP P0AA27
B	343	PRO	-	expression tag	UNP P0AA27
B	453	GLY	-	linker	UNP Q9UHX1
B	454	SER	-	linker	UNP Q9UHX1
B	455	ALA	-	linker	UNP Q9UHX1
B	456	MET	-	linker	UNP Q9UHX1
C	335	MET	-	expression tag	UNP P0AA27
C	336	LYS	-	expression tag	UNP P0AA27
C	337	HIS	-	expression tag	UNP P0AA27
C	338	HIS	-	expression tag	UNP P0AA27
C	339	HIS	-	expression tag	UNP P0AA27
C	340	HIS	-	expression tag	UNP P0AA27
C	341	HIS	-	expression tag	UNP P0AA27
C	342	HIS	-	expression tag	UNP P0AA27
C	343	PRO	-	expression tag	UNP P0AA27
C	453	GLY	-	linker	UNP Q9UHX1
C	454	SER	-	linker	UNP Q9UHX1
C	455	ALA	-	linker	UNP Q9UHX1
C	456	MET	-	linker	UNP Q9UHX1
D	335	MET	-	expression tag	UNP P0AA27
D	336	LYS	-	expression tag	UNP P0AA27
D	337	HIS	-	expression tag	UNP P0AA27
D	338	HIS	-	expression tag	UNP P0AA27
D	339	HIS	-	expression tag	UNP P0AA27
D	340	HIS	-	expression tag	UNP P0AA27
D	341	HIS	-	expression tag	UNP P0AA27
D	342	HIS	-	expression tag	UNP P0AA27
D	343	PRO	-	expression tag	UNP P0AA27
D	453	GLY	-	linker	UNP Q9UHX1
D	454	SER	-	linker	UNP Q9UHX1
D	455	ALA	-	linker	UNP Q9UHX1
D	456	MET	-	linker	UNP Q9UHX1
E	335	MET	-	expression tag	UNP P0AA27
E	336	LYS	-	expression tag	UNP P0AA27
E	337	HIS	-	expression tag	UNP P0AA27

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	338	HIS	-	expression tag	UNP P0AA27
E	339	HIS	-	expression tag	UNP P0AA27
E	340	HIS	-	expression tag	UNP P0AA27
E	341	HIS	-	expression tag	UNP P0AA27
E	342	HIS	-	expression tag	UNP P0AA27
E	343	PRO	-	expression tag	UNP P0AA27
E	453	GLY	-	linker	UNP Q9UHX1
E	454	SER	-	linker	UNP Q9UHX1
E	455	ALA	-	linker	UNP Q9UHX1
E	456	MET	-	linker	UNP Q9UHX1
F	335	MET	-	expression tag	UNP P0AA27
F	336	LYS	-	expression tag	UNP P0AA27
F	337	HIS	-	expression tag	UNP P0AA27
F	338	HIS	-	expression tag	UNP P0AA27
F	339	HIS	-	expression tag	UNP P0AA27
F	340	HIS	-	expression tag	UNP P0AA27
F	341	HIS	-	expression tag	UNP P0AA27
F	342	HIS	-	expression tag	UNP P0AA27
F	343	PRO	-	expression tag	UNP P0AA27
F	453	GLY	-	linker	UNP Q9UHX1
F	454	SER	-	linker	UNP Q9UHX1
F	455	ALA	-	linker	UNP Q9UHX1
F	456	MET	-	linker	UNP Q9UHX1
G	335	MET	-	expression tag	UNP P0AA27
G	336	LYS	-	expression tag	UNP P0AA27
G	337	HIS	-	expression tag	UNP P0AA27
G	338	HIS	-	expression tag	UNP P0AA27
G	339	HIS	-	expression tag	UNP P0AA27
G	340	HIS	-	expression tag	UNP P0AA27
G	341	HIS	-	expression tag	UNP P0AA27
G	342	HIS	-	expression tag	UNP P0AA27
G	343	PRO	-	expression tag	UNP P0AA27
G	453	GLY	-	linker	UNP Q9UHX1
G	454	SER	-	linker	UNP Q9UHX1
G	455	ALA	-	linker	UNP Q9UHX1
G	456	MET	-	linker	UNP Q9UHX1
H	335	MET	-	expression tag	UNP P0AA27
H	336	LYS	-	expression tag	UNP P0AA27
H	337	HIS	-	expression tag	UNP P0AA27
H	338	HIS	-	expression tag	UNP P0AA27
H	339	HIS	-	expression tag	UNP P0AA27
H	340	HIS	-	expression tag	UNP P0AA27

Continued on next page...

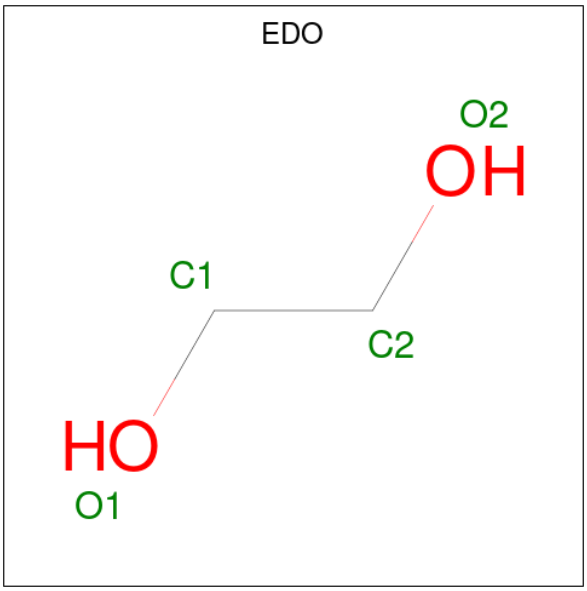
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	341	HIS	-	expression tag	UNP P0AA27
H	342	HIS	-	expression tag	UNP P0AA27
H	343	PRO	-	expression tag	UNP P0AA27
H	453	GLY	-	linker	UNP Q9UHX1
H	454	SER	-	linker	UNP Q9UHX1
H	455	ALA	-	linker	UNP Q9UHX1
H	456	MET	-	linker	UNP Q9UHX1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0

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



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

- Molecule 4 is water.

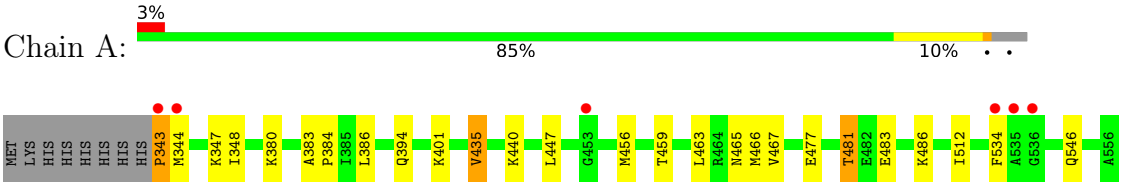
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	148	Total O 148 148	0	0
4	B	132	Total O 132 132	0	0
4	C	173	Total O 173 173	0	0
4	D	123	Total O 123 123	0	0
4	E	149	Total O 149 149	0	0
4	F	156	Total O 156 156	0	0
4	G	141	Total O 141 141	0	0
4	H	169	Total O 169 169	0	0

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.

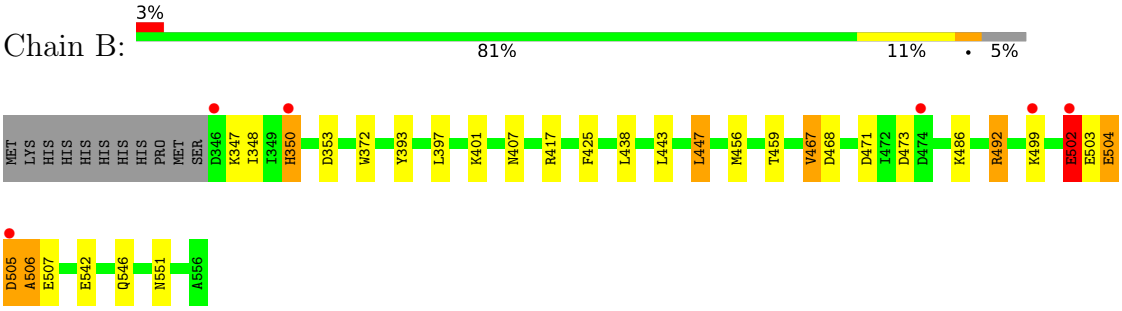
• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

Chain A:



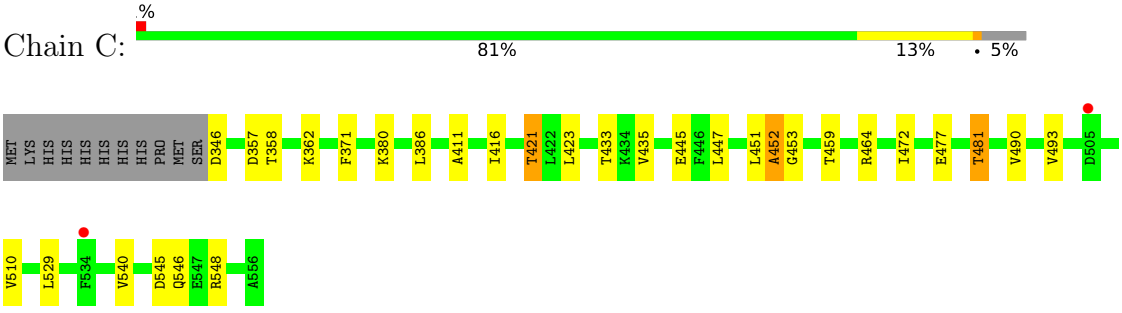
• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

Chain B:



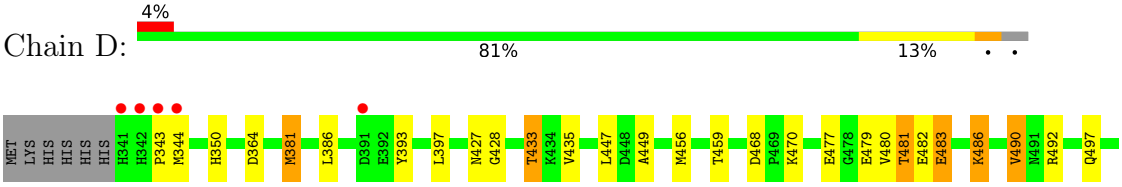
• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

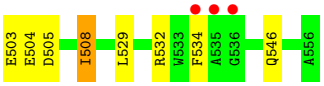
Chain C:



• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

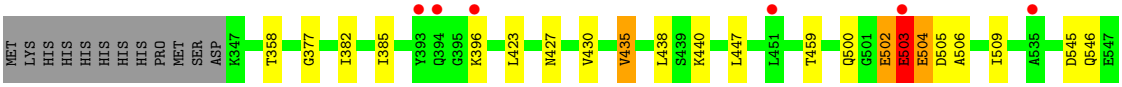
Chain D:





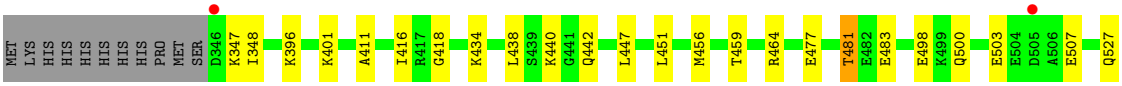
• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

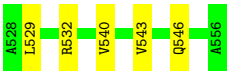
Chain E:



• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

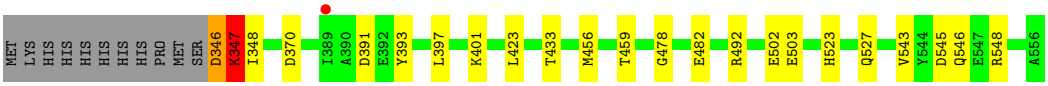
Chain F:





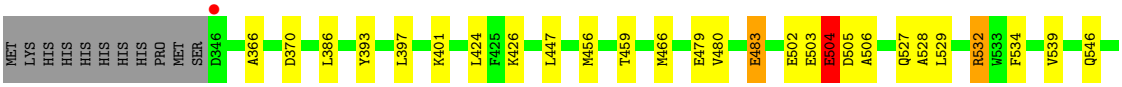
• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

Chain G:



• Molecule 1: thioredoxin N-terminally fused to Puf60(UHM)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.12Å 89.43Å 299.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.20 46.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.75-2.20) 99.8 (46.82-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.271 0.233 , 0.277	Depositor DCC
R_{free} test set	5181 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14337	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 48.23 % 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 8.8621e-05. 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: CL, 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	0.33	0/1682	0.50	0/2272
1	B	0.32	0/1650	0.49	0/2231
1	C	0.33	0/1683	0.51	0/2275
1	D	0.33	0/1712	0.52	0/2314
1	E	0.32	0/1648	0.50	0/2228
1	F	0.34	0/1662	0.51	0/2247
1	G	0.32	0/1656	0.49	0/2239
1	H	0.33	0/1656	0.50	0/2239
All	All	0.33	0/13349	0.50	0/18045

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	E	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	534	PHE	Peptide
1	B	502	GLU	Peptide
1	B	504	GLU	Peptide
1	C	451	LEU	Peptide
1	C	452[A]	ALA	Peptide
1	E	503	GLU	Peptide
1	E	504	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1655	0	1631	14	0
1	B	1624	0	1594	33	0
1	C	1657	0	1615	25	0
1	D	1684	0	1645	28	0
1	E	1622	0	1594	33	0
1	F	1636	0	1601	17	0
1	G	1630	0	1598	19	0
1	H	1630	0	1598	19	0
2	A	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	E	4	0	6	0	0
4	A	148	0	0	3	0
4	B	132	0	0	5	0
4	C	173	0	0	7	0
4	D	123	0	0	3	0
4	E	149	0	0	3	0
4	F	156	0	0	3	0
4	G	141	0	0	1	0
4	H	169	0	0	2	0
All	All	14337	0	12882	176	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 (176) 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:G:346:ASP:N	1:G:347:LYS:HB2	1.36	1.41
1:C:452[B]:ALA:CB	1:C:453[B]:GLY:HA2	1.55	1.34
1:C:452[B]:ALA:HB1	1:C:453[B]:GLY:CA	1.64	1.27
1:E:504:GLU:N	1:E:505:ASP:HB3	1.52	1.24
1:B:502:GLU:HG2	1:D:427:ASN:O	1.40	1.18
1:B:506:ALA:CB	1:B:507:GLU:HA	1.79	1.12
1:B:506:ALA:HB1	1:B:507:GLU:CA	1.80	1.11
1:E:504:GLU:H	1:E:505:ASP:HB3	0.91	1.08
1:E:504:GLU:H	1:E:505:ASP:CB	1.69	1.05
1:E:504:GLU:CB	1:E:505:ASP:HB2	1.88	1.03
1:E:504:GLU:HB2	1:E:505:ASP:HB2	1.43	1.00
1:F:347:LYS:HG3	4:F:708:HOH:O	1.63	0.98
1:H:534:PHE:HB3	4:H:720:HOH:O	1.66	0.94
1:E:504:GLU:N	1:E:505:ASP:CB	2.30	0.93
2:A:1:CL:CL	4:A:695:HOH:O	2.25	0.92
1:G:346:ASP:N	1:G:347:LYS:CB	2.30	0.90
1:B:506:ALA:HB1	1:B:507:GLU:HA	0.91	0.89
1:D:435:VAL:HG13	1:G:456:MET:SD	2.13	0.88
1:D:508:ILE:HB	4:D:672:HOH:O	1.76	0.86
1:C:452[A]:ALA:HB2	4:C:717:HOH:O	1.74	0.86
1:C:380:LYS:HG3	4:C:720:HOH:O	1.74	0.85
1:G:346:ASP:HA	1:G:348:ILE:H	1.41	0.85
1:B:425:PHE:HD1	4:B:681:HOH:O	1.64	0.80
1:C:477:GLU:O	1:C:481:THR:HG23	1.83	0.79
1:G:346:ASP:CA	1:G:347:LYS:HB2	2.14	0.77
1:B:502:GLU:CG	1:D:427:ASN:O	2.30	0.77
1:E:435:VAL:HG13	1:F:456:MET:SD	2.27	0.75
1:A:465:ASN:HB2	4:A:691:HOH:O	1.87	0.75
1:B:505:ASP:O	1:B:506:ALA:HB2	1.86	0.75
1:E:504:GLU:CA	1:E:505:ASP:CB	2.66	0.74
1:E:502:GLU:O	1:E:503:GLU:HG2	1.90	0.71
1:G:347:LYS:HE2	1:G:391:ASP:OD1	1.91	0.71
1:C:445:GLU:HG3	4:C:721:HOH:O	1.91	0.70
1:E:504:GLU:CB	1:E:505:ASP:CB	2.68	0.70
1:E:504:GLU:CG	1:E:505:ASP:HB2	2.22	0.70
1:H:479:GLU:O	1:H:483:GLU:HG2	1.93	0.69
1:B:459:THR:H	1:B:546:GLN:HE21	1.41	0.69
1:B:505:ASP:O	1:B:506:ALA:CB	2.40	0.69
1:A:477:GLU:O	1:A:481:THR:HG22	1.93	0.68
1:C:452[A]:ALA:HB1	1:C:453[A]:GLY:O	1.93	0.68
1:G:423:LEU:HD22	1:G:433:THR:HG22	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:503:GLU:O	1:H:503:GLU:HG3	1.93	0.67
1:G:545:ASP:OD2	1:G:548:ARG:HG3	1.95	0.66
1:A:435:VAL:HG13	1:H:456:MET:SD	2.36	0.66
1:B:456:MET:SD	1:C:435:VAL:HG13	2.35	0.66
1:B:551:ASN:O	1:D:433:THR:HG21	1.96	0.65
1:E:503:GLU:O	1:E:506:ALA:CB	2.44	0.65
1:D:343:PRO:CB	1:D:344:MET:HA	2.27	0.65
1:E:503:GLU:O	1:E:506:ALA:HB2	1.96	0.64
1:D:435:VAL:CG1	1:G:456:MET:SD	2.85	0.64
1:D:459:THR:H	1:D:546:GLN:HE21	1.46	0.64
1:D:381:MET:HB3	4:D:667:HOH:O	1.98	0.63
1:E:430:VAL:HG13	4:E:702:HOH:O	1.98	0.63
1:C:452[B]:ALA:CB	1:C:453[B]:GLY:CA	2.37	0.63
1:F:347:LYS:HE3	4:F:708:HOH:O	1.97	0.63
1:B:417:ARG:NH1	4:B:682:HOH:O	2.31	0.63
1:C:545:ASP:OD2	1:C:548:ARG:HG3	1.99	0.63
1:E:504:GLU:HG3	1:E:505:ASP:HB2	1.81	0.63
1:C:421:THR:HG21	4:G:563:HOH:O	1.97	0.62
1:E:502:GLU:O	1:E:503:GLU:CB	2.47	0.62
1:H:479:GLU:O	1:H:483:GLU:CG	2.47	0.61
1:E:502:GLU:O	1:E:503:GLU:CG	2.48	0.61
1:B:425:PHE:CD1	4:B:681:HOH:O	2.44	0.61
1:H:503:GLU:O	1:H:505:ASP:N	2.33	0.61
1:E:502:GLU:H	1:E:502:GLU:CD	2.04	0.60
1:D:479:GLU:O	1:D:483[A]:GLU:HG2	2.02	0.60
1:D:529:LEU:HD22	1:D:534:PHE:HZ	1.66	0.59
1:C:452[B]:ALA:HB1	1:C:453[B]:GLY:HA2	0.69	0.59
1:F:459:THR:H	1:F:546:GLN:HE21	1.50	0.59
1:B:499:LYS:HD2	1:D:428:GLY:HA3	1.85	0.58
1:A:459:THR:H	1:A:546:GLN:HE21	1.51	0.58
1:B:499:LYS:HD3	1:B:502:GLU:CD	2.24	0.58
1:G:346:ASP:HA	1:G:348:ILE:N	2.16	0.57
1:E:504:GLU:HB2	1:E:505:ASP:CB	2.26	0.57
1:D:456:MET:HE2	1:F:418:GLY:HA3	1.88	0.56
1:B:467:VAL:HG22	1:B:471:ASP:HB2	1.88	0.56
1:D:477:GLU:O	1:D:481:THR:HG23	2.05	0.56
1:F:477:GLU:O	1:F:481:THR:HG23	2.06	0.56
1:C:452[A]:ALA:CA	4:C:717:HOH:O	2.53	0.55
1:G:459:THR:H	1:G:546:GLN:HE21	1.54	0.55
1:E:545:ASP:OD2	1:E:548:ARG:HG3	2.07	0.55
1:H:459:THR:H	1:H:546:GLN:HE21	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLU:CG	1:B:503:GLU:HA	2.38	0.54
1:C:358:THR:HG22	4:C:579:HOH:O	2.06	0.54
1:G:346:ASP:CA	1:G:347:LYS:CB	2.79	0.53
1:B:492:ARG:HD2	4:B:677:HOH:O	2.08	0.53
1:C:423:LEU:HD22	1:C:433:THR:HG22	1.90	0.53
1:H:504:GLU:HG3	1:H:505:ASP:N	2.24	0.53
1:E:459:THR:H	1:E:546:GLN:HE21	1.55	0.53
1:B:551:ASN:O	1:D:433:THR:CG2	2.57	0.52
1:E:502:GLU:CD	1:E:502:GLU:N	2.63	0.52
1:C:472:ILE:HD11	1:C:510:VAL:HG21	1.92	0.52
1:H:393:TYR:HB3	1:H:397:LEU:HB3	1.92	0.52
1:B:502:GLU:HG3	1:B:503:GLU:CB	2.40	0.51
1:H:503:GLU:HG3	1:H:506:ALA:HB2	1.93	0.51
1:D:497:GLN:HB3	1:D:508:ILE:HD11	1.93	0.50
1:G:347:LYS:CE	1:G:391:ASP:OD1	2.60	0.50
1:E:423:LEU:HB3	4:E:702:HOH:O	2.10	0.50
1:B:459:THR:H	1:B:546:GLN:NE2	2.09	0.49
1:E:503:GLU:HG3	1:E:504:GLU:N	2.27	0.49
1:F:477:GLU:O	1:F:481:THR:CG2	2.60	0.49
1:C:459:THR:H	1:C:546:GLN:HE21	1.59	0.49
1:B:348:ILE:HG21	1:B:401:LYS:HG3	1.94	0.49
1:D:459:THR:H	1:D:546:GLN:NE2	2.08	0.49
1:E:377:GLY:HA3	1:F:396:LYS:HE2	1.95	0.49
1:E:500:GLN:NE2	1:E:509:ILE:HG12	2.27	0.49
1:B:438:LEU:N	1:B:438:LEU:HD23	2.27	0.49
1:H:503:GLU:O	1:H:506:ALA:N	2.37	0.48
1:F:401:LYS:NZ	4:F:703:HOH:O	2.36	0.48
1:H:426:LYS:HB2	4:H:711:HOH:O	2.13	0.48
1:B:502:GLU:CD	1:B:503:GLU:HA	2.34	0.48
1:G:523:HIS:O	1:G:527:GLN:HG3	2.14	0.47
1:H:480:VAL:HA	1:H:483:GLU:HG3	1.97	0.47
1:F:347:LYS:HG3	1:F:348:ILE:H	1.80	0.47
1:H:528:ALA:O	1:H:532:ARG:HD2	2.14	0.47
1:D:449:ALA:HB2	4:D:675:HOH:O	2.13	0.47
1:G:459:THR:H	1:G:546:GLN:NE2	2.12	0.47
1:C:371:PHE:HE1	1:C:423:LEU:HG	1.79	0.47
1:F:498:GLU:OE1	1:F:500:GLN:NE2	2.48	0.47
1:A:348:ILE:HG21	1:A:401:LYS:HG3	1.97	0.46
1:E:358:THR:HG22	4:E:680:HOH:O	2.15	0.46
1:G:370:ASP:HB3	1:G:401:LYS:HG2	1.97	0.46
1:E:502:GLU:O	1:E:503:GLU:HB3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:GLU:C	1:D:505:ASP:H	2.19	0.46
1:F:434:LYS:HG2	1:F:438:LEU:HD22	1.97	0.46
1:E:382:ILE:HA	1:E:385:ILE:HD12	1.98	0.45
1:D:393:TYR:HB3	1:D:397:LEU:HB3	1.98	0.45
1:F:438:LEU:HG	1:F:442:GLN:HB2	1.97	0.45
1:H:466:MET:HA	1:H:539:VAL:HG22	1.99	0.45
1:A:347:LYS:HG2	1:A:394:GLN:HE21	1.82	0.45
1:A:343:PRO:N	1:A:344:MET:HA	2.32	0.45
1:H:370:ASP:HB3	1:H:401:LYS:HG2	1.99	0.44
1:B:499:LYS:HD3	1:B:502:GLU:OE1	2.17	0.44
1:E:438:LEU:HD23	1:E:438:LEU:N	2.32	0.44
1:A:465:ASN:CB	4:A:691:HOH:O	2.54	0.44
1:B:502:GLU:HG3	1:B:503:GLU:CA	2.48	0.44
1:H:366:ALA:HB1	1:H:424:LEU:HD11	2.00	0.44
1:C:357:ASP:OD1	1:C:362:LYS:HE2	2.18	0.44
1:D:343:PRO:HB2	1:D:344:MET:HA	1.99	0.44
1:G:393:TYR:HB3	1:G:397:LEU:HB3	2.00	0.43
1:C:452[B]:ALA:N	4:C:717:HOH:O	2.51	0.43
1:B:502:GLU:HG3	1:B:503:GLU:HA	2.00	0.43
1:D:486:LYS:HB2	1:D:486:LYS:HE2	1.57	0.43
1:H:503:GLU:CG	1:H:506:ALA:HB2	2.49	0.43
1:B:353:ASP:H	1:B:407:ASN:ND2	2.17	0.43
1:A:483:GLU:O	1:A:486:LYS:HG2	2.19	0.42
1:G:503:GLU:CD	1:G:503:GLU:H	2.23	0.42
1:F:447:LEU:O	1:F:451:LEU:HB2	2.19	0.42
1:A:456:MET:HE2	1:A:456:MET:HB3	1.96	0.42
1:B:443:LEU:O	1:B:447:LEU:HD22	2.19	0.42
1:C:452[A]:ALA:N	4:C:717:HOH:O	2.52	0.42
1:A:466:MET:HG2	1:A:467:VAL:HG23	2.00	0.42
1:B:393:TYR:HB3	1:B:397:LEU:HB3	2.01	0.42
1:D:481:THR:HB	1:D:490:VAL:HG21	2.01	0.42
1:C:464:ARG:HB2	1:C:540:VAL:HB	2.01	0.42
1:C:472:ILE:HD11	1:C:510:VAL:CG2	2.49	0.42
1:B:350:HIS:CE1	1:B:372:TRP:HE1	2.37	0.42
1:D:477:GLU:O	1:D:481:THR:CG2	2.67	0.42
1:A:463:LEU:HB2	1:A:512:ILE:HB	2.01	0.42
1:B:350:HIS:HE1	1:B:372:TRP:HE1	1.67	0.42
1:D:508:ILE:C	1:D:508:ILE:HD13	2.40	0.42
1:E:504:GLU:HG3	1:E:505:ASP:CB	2.48	0.42
1:C:481:THR:HG22	1:C:493:VAL:HG21	2.02	0.41
1:D:470:LYS:HE3	1:D:470:LYS:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:GLU:HG3	1:E:504:GLU:H	1.86	0.41
1:C:411:ALA:HB1	1:C:416:ILE:HB	2.03	0.41
1:B:473:ASP:HB2	4:B:680:HOH:O	2.20	0.41
1:A:486:LYS:HB3	1:A:486:LYS:HE2	1.82	0.41
1:A:383:ALA:HB3	1:A:384:PRO:HD3	2.03	0.40
1:D:497:GLN:CB	1:D:508:ILE:HD11	2.51	0.40
1:E:427:ASN:HD22	1:H:502:GLU:HB2	1.85	0.40
1:D:480:VAL:O	1:D:483[A]:GLU:HG3	2.21	0.40
1:F:411:ALA:HB1	1:F:416:ILE:HB	2.04	0.40
1:F:464:ARG:HB2	1:F:540:VAL:HB	2.03	0.40
1:F:348:ILE:HG21	1:F:401:LYS:HG3	2.02	0.40
1:G:478:GLY:O	1:G:482:GLU:HG2	2.22	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	212/222 (96%)	209 (99%)	3 (1%)	0	100 100
1	B	210/222 (95%)	202 (96%)	5 (2%)	3 (1%)	11 8
1	C	213/222 (96%)	206 (97%)	7 (3%)	0	100 100
1	D	216/222 (97%)	208 (96%)	7 (3%)	1 (0%)	29 31
1	E	208/222 (94%)	203 (98%)	4 (2%)	1 (0%)	29 31
1	F	210/222 (95%)	208 (99%)	2 (1%)	0	100 100
1	G	209/222 (94%)	205 (98%)	3 (1%)	1 (0%)	29 31
1	H	209/222 (94%)	204 (98%)	4 (2%)	1 (0%)	29 31
All	All	1687/1776 (95%)	1645 (98%)	35 (2%)	7 (0%)	34 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	GLU
1	B	504	GLU
1	B	506	ALA
1	H	504	GLU
1	E	503	GLU
1	G	347	LYS
1	D	504	GLU

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	177/185 (96%)	171 (97%)	6 (3%)	37 47
1	B	170/185 (92%)	160 (94%)	10 (6%)	19 23
1	C	175/185 (95%)	168 (96%)	7 (4%)	31 40
1	D	179/185 (97%)	162 (90%)	17 (10%)	8 8
1	E	172/185 (93%)	167 (97%)	5 (3%)	42 54
1	F	173/185 (94%)	164 (95%)	9 (5%)	23 28
1	G	173/185 (94%)	168 (97%)	5 (3%)	42 54
1	H	173/185 (94%)	166 (96%)	7 (4%)	31 40
All	All	1392/1480 (94%)	1326 (95%)	66 (5%)	27 33

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	LYS
1	A	386	LEU
1	A	435	VAL
1	A	440	LYS
1	A	447	LEU
1	A	481	THR
1	B	347[A]	LYS
1	B	347[B]	LYS
1	B	350	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	447	LEU
1	B	467	VAL
1	B	468	ASP
1	B	486	LYS
1	B	492	ARG
1	B	505	ASP
1	B	542	GLU
1	C	346	ASP
1	C	386	LEU
1	C	421	THR
1	C	447	LEU
1	C	481	THR
1	C	490	VAL
1	C	529	LEU
1	D	350[A]	HIS
1	D	350[B]	HIS
1	D	364	ASP
1	D	381	MET
1	D	386	LEU
1	D	433	THR
1	D	447	LEU
1	D	468	ASP
1	D	481	THR
1	D	482	GLU
1	D	483[A]	GLU
1	D	483[B]	GLU
1	D	486	LYS
1	D	490	VAL
1	D	492	ARG
1	D	508	ILE
1	D	532	ARG
1	E	396	LYS
1	E	435	VAL
1	E	440	LYS
1	E	447	LEU
1	E	502	GLU
1	F	440	LYS
1	F	481	THR
1	F	483	GLU
1	F	503	GLU
1	F	507	GLU
1	F	527	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	529	LEU
1	F	532	ARG
1	F	543	VAL
1	G	346	ASP
1	G	347	LYS
1	G	492	ARG
1	G	502	GLU
1	G	543	VAL
1	H	386	LEU
1	H	447	LEU
1	H	483	GLU
1	H	504	GLU
1	H	527	GLN
1	H	529	LEU
1	H	532	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	500	GLN
1	A	527	GLN
1	A	546	GLN
1	B	394	GLN
1	B	407	ASN
1	B	546	GLN
1	C	350	HIS
1	C	546	GLN
1	D	497	GLN
1	D	523	HIS
1	D	546	GLN
1	E	407	ASN
1	E	427	ASN
1	E	546	GLN
1	F	546	GLN
1	G	500	GLN
1	G	546	GLN
1	H	546	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)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	E	557	-	3,3,3	0.51	0	2,2,2	0.20	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	E	557	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	557	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	214/222 (96%)	-0.10	6 (2%)	53	51	12, 18, 25, 31	0
1	B	211/222 (95%)	0.03	6 (2%)	53	51	12, 23, 30, 32	0
1	C	211/222 (95%)	-0.15	2 (0%)	84	83	12, 18, 24, 27	0
1	D	216/222 (97%)	0.11	8 (3%)	41	39	15, 22, 28, 32	0
1	E	210/222 (94%)	0.04	6 (2%)	51	49	12, 20, 29, 32	0
1	F	211/222 (95%)	0.01	2 (0%)	84	83	10, 19, 28, 36	0
1	G	211/222 (95%)	-0.05	1 (0%)	91	90	12, 22, 28, 32	0
1	H	211/222 (95%)	-0.05	1 (0%)	91	90	11, 19, 26, 32	0
All	All	1695/1776 (95%)	-0.02	32 (1%)	66	65	10, 20, 28, 36	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	HIS	9.7
1	B	346	ASP	5.4
1	F	505	ASP	4.6
1	F	346	ASP	4.5
1	D	534	PHE	3.2
1	D	342	HIS	3.2
1	A	453	GLY	3.2
1	D	344	MET	3.1
1	A	534	PHE	3.0
1	D	535	ALA	2.9
1	D	343	PRO	2.8
1	C	505	ASP	2.7
1	A	343	PRO	2.7
1	A	344	MET	2.6
1	B	474	ASP	2.5
1	A	535	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	350	HIS	2.5
1	E	396	LYS	2.5
1	E	503	GLU	2.4
1	E	535	ALA	2.4
1	B	502	GLU	2.4
1	D	391	ASP	2.4
1	E	394	GLN	2.4
1	E	451	LEU	2.4
1	B	505	ASP	2.2
1	B	499	LYS	2.2
1	D	536	GLY	2.2
1	C	534	PHE	2.2
1	A	536	GLY	2.1
1	G	389	ILE	2.1
1	E	393	TYR	2.1
1	H	346	ASP	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	557	4/4	0.72	0.26	32,33,33,33	0
2	CL	F	1	1/1	0.81	0.12	45,45,45,45	0
2	CL	E	1	1/1	0.88	0.10	46,46,46,46	0
2	CL	A	1	1/1	0.94	0.08	37,37,37,37	0
2	CL	H	1	1/1	0.95	0.11	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.