Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 04:43 PM EDT

PDB ID	:	4HUW
Title	:	Crystal Structure of H2Db-NPM6T
Authors	:	Gras, S.; Twist, K.A.; Rossjohn, J.
Deposited on	:	2012-11-04
Resolution	:	3.16 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:

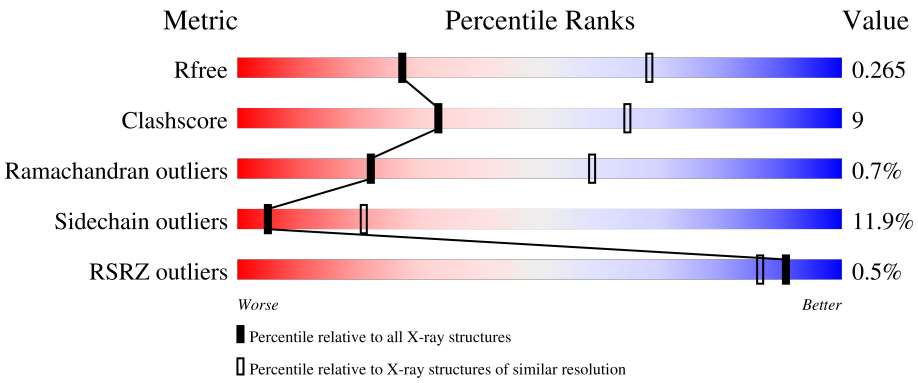
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	281	71% 24% • •
1	C	281	72% 23% • •
1	E	281	66% 31% • •
1	G	281	71% 25% • •
2	B	100	2% 72% 26% •

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Mol	Chain	Length	Quality of chain
2	D	100	%, 70%, 29%
2	F	100	3%, 76%, 23%
2	H	100	2%, 77%, 21%
3	I	9	89%, 11%
3	J	9	89%, 11%
3	K	9	89%, 11%
3	L	9	67%, 22%, 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12981 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2303	1453	412	429	9	0	3	0
1	C	277	2292	1447	408	428	9	1	2	0
1	E	277	2292	1447	408	428	9	0	2	0
1	G	277	2282	1441	405	427	9	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01899
C	0	MET	-	initiating methionine	UNP P01899
E	0	MET	-	initiating methionine	UNP P01899
G	0	MET	-	initiating methionine	UNP P01899

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	826	528	139	151	8	2	0	0
2	D	100	826	528	139	151	8	1	0	0
2	F	100	826	528	139	151	8	2	0	0
2	H	100	826	528	139	151	8	2	0	0

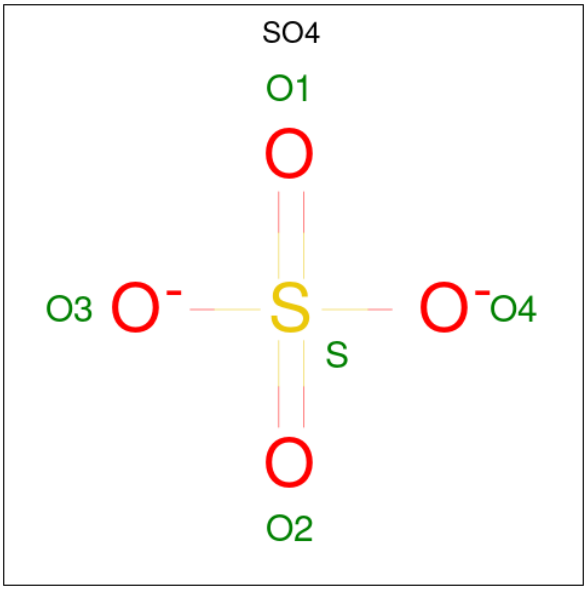
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01887
D	0	MET	-	initiating methionine	UNP P01887
F	0	MET	-	initiating methionine	UNP P01887
H	0	MET	-	initiating methionine	UNP P01887

- Molecule 3 is a protein called NPM6T variant peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	9	68	37	11	19	1	0	0	0
3	J	9	68	37	11	19	1	0	0	0
3	K	9	68	37	11	19	1	0	0	0
3	L	9	68	37	11	19	1	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	E	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	G	1	5	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	38	38	38	0	0
5	B	17	17	17	0	0
5	C	45	45	45	0	0
5	D	14	14	14	0	0
5	E	33	33	33	0	0
5	F	7	7	7	0	0
5	G	39	39	39	0	0
5	H	12	12	12	0	0
5	I	1	1	1	0	0
5	J	2	2	2	0	0
5	K	2	2	2	0	0
5	L	1	1	1	0	0

3 Residue-property plots (i)

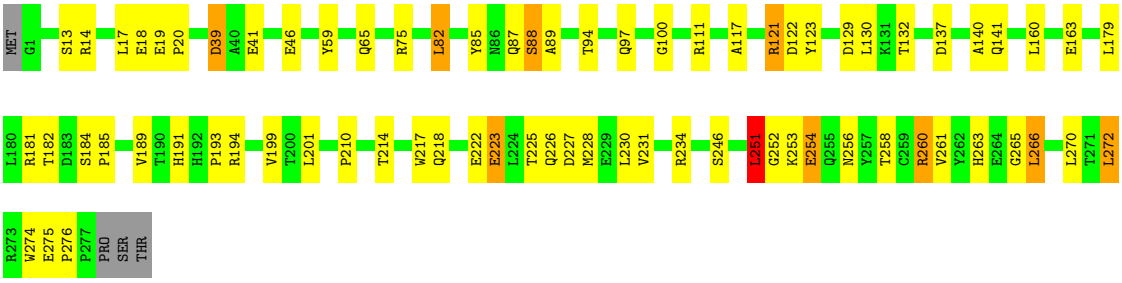
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:

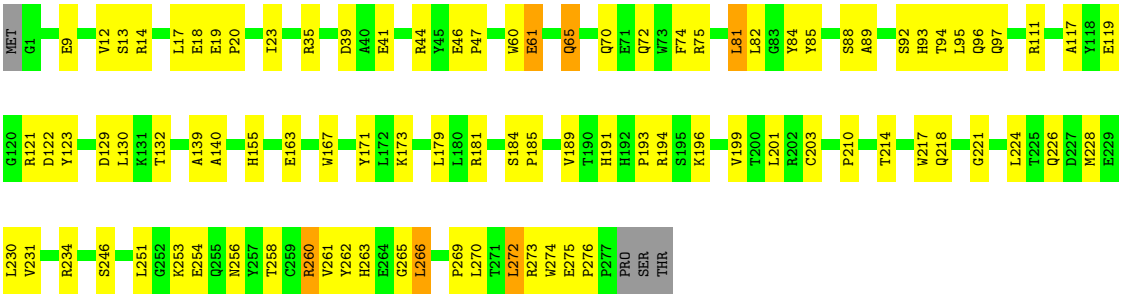
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain C:



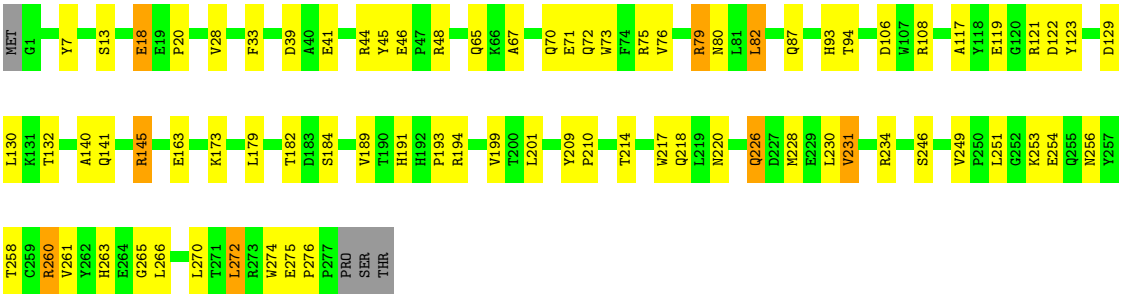
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain E:



• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain G: 71% 25%

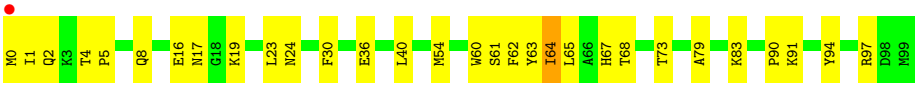


• Molecule 2: Beta-2-microglobulin

Chain B: 2% 72% 26%

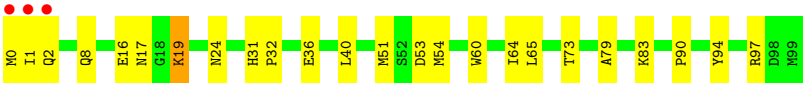
• Molecule 2: Beta-2-microglobulin

Chain D: % 70% 29%



• Molecule 2: Beta-2-microglobulin

Chain F: 3% 76% 23%



• Molecule 2: Beta-2-microglobulin

Chain H: 2% 77% 21%

• Molecule 3: NPM6T variant peptide

Chain I: 89% 11%

• Molecule 3: NPM6T variant peptide

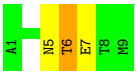
Chain J: 89% 11%

• Molecule 3: NPM6T variant peptide

Chain K: 89% 11%

• Molecule 3: NPM6T variant peptide

Chain L: 67% 22% 11%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.93Å 84.68Å 136.42Å 90.00° 90.93° 90.00°	Depositor
Resolution (Å)	58.12 – 3.16 58.12 – 3.16	Depositor EDS
% Data completeness (in resolution range)	98.6 (58.12-3.16) 98.9 (58.12-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.178 , 0.247 0.192 , 0.265	Depositor DCC
R_{free} test set	1565 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12981	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 26.37 % 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 2.6673e-03. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.52	0/2372	0.77	0/3221
1	C	0.54	0/2361	0.76	0/3207
1	E	0.51	0/2361	0.75	0/3207
1	G	0.51	0/2350	0.74	0/3192
2	B	0.54	0/852	0.73	0/1154
2	D	0.54	0/852	0.72	0/1154
2	F	0.51	0/852	0.73	0/1154
2	H	0.55	0/852	0.71	0/1154
3	I	0.55	0/67	0.73	0/88
3	J	0.59	0/67	0.71	0/88
3	K	0.64	0/67	0.74	0/88
3	L	0.60	0/67	0.82	0/88
All	All	0.53	0/13120	0.75	0/17795

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 (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	2303	0	2173	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2292	0	2161	39	0
1	E	2292	0	2161	48	0
1	G	2282	0	2155	46	0
2	B	826	0	806	18	0
2	D	826	0	806	23	0
2	F	826	0	806	19	0
2	H	826	0	806	19	0
3	I	68	0	59	1	0
3	J	68	0	59	2	0
3	K	68	0	59	2	0
3	L	68	0	59	9	0
4	A	10	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	A	38	0	0	1	0
5	B	17	0	0	0	0
5	C	45	0	0	1	0
5	D	14	0	0	1	0
5	E	33	0	0	0	0
5	F	7	0	0	0	0
5	G	39	0	0	1	0
5	H	12	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
All	All	12981	0	12110	215	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 9.

All (215) 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:H:64:ILE:CD1	2:H:64:ILE:CG1	1.78	1.56
1:C:121:ARG:HG2	2:D:1:ILE:HG13	1.42	0.99
2:F:2:GLN:HE21	1:G:121:ARG:NH2	1.67	0.91
2:F:2:GLN:HE21	1:G:121:ARG:HH22	1.07	0.91
1:C:87:GLN:O	1:C:89:ALA:N	2.07	0.88
1:C:97:GLN:HE22	3:J:5:ASN:HD21	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ARG:HG3	2:H:1:ILE:HG13	1.61	0.82
1:E:193:PRO:HA	1:E:199:VAL:HG12	1.62	0.82
1:A:121:ARG:HG3	2:B:1:ILE:HG13	1.62	0.81
1:C:14:ARG:HD3	1:C:17:LEU:HD12	1.64	0.79
1:C:193:PRO:HA	1:C:199:VAL:HG12	1.63	0.78
1:A:82:LEU:HD11	1:A:89:ALA:H	1.50	0.76
1:A:89:ALA:HB3	1:A:93:HIS:NE2	2.01	0.76
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.22	0.75
1:A:121:ARG:HH22	2:D:2:GLN:HB2	1.52	0.74
1:G:70:GLN:HE22	3:K:5:ASN:H	1.37	0.73
2:F:2:GLN:NE2	1:G:121:ARG:HH22	1.86	0.71
1:G:234:ARG:HH11	2:H:8:GLN:HE21	1.37	0.71
1:E:121:ARG:HG3	2:F:1:ILE:HG13	1.71	0.71
1:A:267:PRO:HD2	5:A:427:HOH:O	1.90	0.70
1:G:76:VAL:HG12	1:G:80:ASN:HD21	1.60	0.67
1:C:191:HIS:CE1	1:C:199:VAL:HG11	2.31	0.65
1:E:97:GLN:HE22	3:L:5:ASN:HD21	1.45	0.65
1:C:121:ARG:CG	2:D:1:ILE:HG13	2.24	0.64
1:E:14:ARG:HD3	1:E:17:LEU:HD12	1.79	0.63
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.33	0.62
1:C:234:ARG:HH11	2:D:8:GLN:HE21	1.48	0.62
1:G:70:GLN:NE2	3:K:5:ASN:H	1.98	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.35	0.61
1:C:121:ARG:NH2	1:C:137:ASP:OD2	2.33	0.61
1:A:121:ARG:NH2	2:D:2:GLN:HB2	2.16	0.60
1:C:85:TYR:O	1:C:87:GLN:HG3	2.02	0.60
2:F:17:ASN:HD21	2:F:97:ARG:HH22	1.50	0.60
1:E:13:SER:HB3	1:E:93:HIS:H	1.67	0.59
2:B:17:ASN:HD21	2:B:97:ARG:HH22	1.50	0.59
2:H:24:ASN:HB3	2:H:65:LEU:HD11	1.85	0.58
1:A:234:ARG:HH11	2:B:8:GLN:HE21	1.52	0.58
1:E:155[B]:HIS:HB2	3:L:6:THR:HG21	1.85	0.58
2:F:2:GLN:NE2	1:G:121:ARG:NH2	2.48	0.58
1:G:87:GLN:HE21	1:G:93:HIS:CE1	2.21	0.58
1:E:155[A]:HIS:CD2	3:L:6:THR:HG22	2.40	0.57
1:E:231:VAL:HB	2:F:8:GLN:HE22	1.70	0.57
1:C:97:GLN:HE22	3:J:5:ASN:ND2	2.00	0.57
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.87	0.57
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.86	0.57
1:G:119:GLU:O	2:H:1:ILE:HB	2.05	0.56
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.88	0.56
1:A:121:ARG:HH21	2:D:2:GLN:HE21	1.54	0.56
2:D:16:GLU:HB3	2:D:19:LYS:HB2	1.87	0.56
2:D:17:ASN:HD21	2:D:97:ARG:HH22	1.52	0.55
1:E:189:VAL:HG23	1:E:272:LEU:HD12	1.88	0.55
1:A:87:GLN:O	1:A:88:SER:C	2.44	0.55
1:C:20:PRO:HD2	1:C:75[B]:ARG:HG2	1.88	0.54
1:G:189:VAL:HG23	1:G:272:LEU:HD12	1.89	0.54
2:B:23:LEU:O	2:B:67:HIS:HA	2.07	0.54
1:E:201:LEU:O	1:E:246:SER:HA	2.08	0.54
1:E:70:GLN:HE22	3:L:5:ASN:ND2	2.06	0.54
1:C:252:GLY:C	1:C:254:GLU:H	2.11	0.54
1:A:234:ARG:HD3	2:B:8:GLN:NE2	2.23	0.53
1:C:218:GLN:HG2	1:C:223:GLU:HA	1.90	0.53
1:C:201:LEU:O	1:C:246:SER:HA	2.08	0.53
2:F:16:GLU:HB3	2:F:19:LYS:HB2	1.91	0.53
1:G:218:GLN:HG3	1:G:260:ARG:HH12	1.74	0.53
1:G:201:LEU:O	1:G:246:SER:HA	2.09	0.53
1:C:189:VAL:HG23	1:C:272:LEU:HD12	1.91	0.53
1:C:210:PRO:O	1:C:263:HIS:HE1	1.92	0.52
1:E:72:GLN:HE22	1:E:75[B]:ARG:CZ	2.22	0.52
1:G:123:TYR:CZ	1:G:140:ALA:HA	2.44	0.52
1:C:14:ARG:NH2	1:C:39:ASP:OD1	2.43	0.52
1:A:23:ILE:HD12	2:B:54:MET:SD	2.50	0.51
1:A:156:TYR:HE1	3:I:5:ASN:HD22	1.58	0.51
1:E:123:TYR:CZ	1:E:140:ALA:HA	2.45	0.51
1:C:111:ARG:HD2	5:C:402:HOH:O	2.10	0.51
1:E:210:PRO:O	1:E:263:HIS:HE1	1.94	0.51
1:G:75[A]:ARG:HH21	1:G:79:ARG:HH22	1.59	0.51
1:C:123:TYR:CZ	1:C:140:ALA:HA	2.45	0.51
1:G:70:GLN:O	1:G:73:TRP:N	2.44	0.51
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.45	0.51
1:A:201:LEU:O	1:A:246:SER:HA	2.10	0.51
1:G:79:ARG:O	1:G:82:LEU:HB2	2.11	0.51
1:E:167:TRP:HB3	1:E:171:TYR:HE2	1.74	0.51
1:C:251:LEU:HD21	2:H:94:TYR:OH	2.12	0.50
2:D:91:LYS:HG2	5:D:113:HOH:O	2.11	0.50
1:G:191:HIS:CE1	1:G:199:VAL:HG11	2.47	0.50
1:G:234:ARG:HD3	2:H:8:GLN:NE2	2.26	0.49
1:G:76:VAL:HG12	1:G:80:ASN:ND2	2.25	0.49
2:B:83:LYS:HG2	2:B:90:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HD21	1:C:88:SER:HA	1.95	0.49
1:C:217:TRP:HB2	1:C:228:MET:HE2	1.95	0.49
2:D:23:LEU:O	2:D:67:HIS:HA	2.13	0.49
1:A:218:GLN:HG3	1:A:260:ARG:HH12	1.77	0.48
1:A:199:VAL:HG13	1:A:251:LEU:HD22	1.95	0.48
1:E:47:PRO:HG3	1:E:60:TRP:CZ2	2.49	0.48
1:G:210:PRO:O	1:G:263:HIS:HE1	1.97	0.48
1:A:129:ASP:OD2	1:A:132:THR:HG22	2.13	0.48
1:C:218:GLN:HG3	1:C:260:ARG:HH12	1.79	0.48
1:E:61:GLU:OE2	1:E:65:GLN:NE2	2.47	0.48
1:G:217:TRP:H	1:G:228:MET:HE1	1.78	0.48
1:G:20:PRO:HD2	1:G:75[B]:ARG:HG2	1.94	0.48
2:H:83:LYS:HG2	2:H:90:PRO:HG3	1.96	0.48
2:B:16:GLU:HB3	2:B:19:LYS:HB2	1.96	0.47
1:G:71:GLU:O	1:G:75[B]:ARG:HG3	2.13	0.47
2:H:4:THR:HA	2:H:5:PRO:HD3	1.87	0.47
1:A:100:GLY:O	1:A:160:LEU:HD22	2.14	0.47
1:A:210:PRO:O	1:A:263:HIS:HE1	1.97	0.47
1:E:85:TYR:CZ	1:E:139:ALA:HB3	2.49	0.47
1:C:231:VAL:HB	2:D:8:GLN:HE22	1.80	0.47
1:E:263:HIS:CD2	1:E:265:GLY:H	2.32	0.47
2:F:83:LYS:HG2	2:F:90:PRO:HG3	1.96	0.47
1:A:19:GLU:HB3	1:A:75[B]:ARG:NH2	2.30	0.47
1:C:263:HIS:CD2	1:C:265:GLY:H	2.32	0.47
1:C:129:ASP:OD2	1:C:132:THR:HG22	2.15	0.47
1:G:193:PRO:HA	1:G:199:VAL:HG12	1.97	0.47
2:B:17:ASN:HD21	2:B:97:ARG:NH2	2.13	0.47
2:B:38:GLN:HG2	2:B:45:LYS:HD2	1.97	0.47
1:A:231:VAL:HB	2:B:8:GLN:HE22	1.80	0.46
2:D:63:TYR:O	2:D:64:ILE:HD12	2.15	0.46
1:G:129:ASP:OD2	1:G:132:THR:HG22	2.15	0.46
1:E:218:GLN:HG3	1:E:260:ARG:HH12	1.80	0.46
1:G:72:GLN:HE22	1:G:75[B]:ARG:NH1	2.12	0.46
1:G:263:HIS:CD2	1:G:265:GLY:H	2.33	0.46
1:A:75[A]:ARG:HH21	1:A:76:VAL:HG22	1.80	0.46
1:C:87:GLN:C	1:C:89:ALA:H	2.10	0.46
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.51	0.46
1:E:35:ARG:NH1	2:F:53:ASP:HB3	2.31	0.46
1:A:263:HIS:CD2	1:A:265:GLY:H	2.33	0.46
1:C:59:TYR:CD1	1:C:59:TYR:C	2.89	0.46
1:E:261:VAL:HB	1:E:270:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:GLU:O	1:G:20:PRO:HD3	2.16	0.46
1:E:9:GLU:OE1	1:E:70:GLN:NE2	2.45	0.46
1:E:185:PRO:HD2	1:E:266:LEU:HD13	1.98	0.46
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.51	0.46
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.98	0.46
1:C:252:GLY:N	1:C:254:GLU:OE2	2.47	0.46
1:E:121:ARG:NH2	2:H:0:MET:O	2.49	0.46
2:D:30:PHE:CE1	2:D:62:PHE:HB2	2.51	0.46
2:F:79:ALA:HB2	2:F:94:TYR:CD1	2.51	0.46
1:E:191:HIS:CE1	1:E:199:VAL:HG11	2.51	0.45
2:B:63:TYR:O	2:B:64:ILE:HD12	2.16	0.45
2:D:83:LYS:HG2	2:D:90:PRO:HG3	1.96	0.45
2:H:38:GLN:HG2	2:H:45:LYS:HD2	1.98	0.45
1:A:249:VAL:HB	1:A:257:TYR:CE1	2.50	0.45
2:F:17:ASN:HD21	2:F:97:ARG:NH2	2.13	0.45
2:D:79:ALA:HB2	2:D:94:TYR:CD1	2.52	0.45
1:E:217:TRP:H	1:E:228:MET:HE1	1.80	0.45
3:L:6:THR:OG1	3:L:7:GLU:N	2.48	0.45
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.99	0.45
2:D:17:ASN:HD21	2:D:97:ARG:NH2	2.15	0.45
1:E:84:TYR:HB3	1:E:139:ALA:HB1	1.98	0.45
1:E:121:ARG:NH2	2:H:2:GLN:HE21	2.15	0.45
2:B:79:ALA:HB2	2:B:94:TYR:CD1	2.52	0.45
1:E:155[A]:HIS:HB3	3:L:6:THR:HG21	1.98	0.45
1:G:209:TYR:HD1	1:G:210:PRO:HA	1.79	0.45
1:G:45:TYR:CE2	1:G:67:ALA:HB2	2.52	0.45
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.98	0.44
1:A:19:GLU:HB3	1:A:75[B]:ARG:HH21	1.83	0.44
1:C:19:GLU:HB3	1:C:75[B]:ARG:CZ	2.47	0.44
1:C:261:VAL:HB	1:C:270:LEU:HB2	1.99	0.44
1:G:72:GLN:O	1:G:76:VAL:HG23	2.17	0.44
1:G:182:THR:HG22	1:G:210:PRO:HD3	1.99	0.44
1:A:218:GLN:HE21	1:A:260:ARG:HH22	1.65	0.44
1:A:274:TRP:O	1:A:276:PRO:HD3	2.18	0.44
1:E:20:PRO:HD3	1:E:75[B]:ARG:HB3	2.00	0.44
1:E:196:LYS:H	1:E:196:LYS:HZ3	1.66	0.44
1:G:261:VAL:HB	1:G:270:LEU:HB2	2.00	0.44
2:B:1:ILE:HD13	2:D:1:ILE:HD13	2.00	0.44
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.53	0.43
1:E:129:ASP:OD2	1:E:132:THR:HG22	2.18	0.43
2:D:54:MET:HA	2:D:64:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLN:C	1:C:228:MET:H	2.21	0.43
1:G:7:TYR:HH	1:G:33:PHE:HZ	1.64	0.43
1:A:217:TRP:H	1:A:228:MET:HE1	1.84	0.43
1:C:191:HIS:NE2	1:C:199:VAL:HG21	2.32	0.43
1:A:108:ARG:HD3	1:E:262:TYR:CD2	2.53	0.43
1:G:274:TRP:O	1:G:276:PRO:HD3	2.18	0.43
1:C:185:PRO:HD2	1:C:266:LEU:HD13	2.00	0.43
1:E:97:GLN:HE22	3:L:5:ASN:ND2	2.14	0.43
1:C:182:THR:HG22	1:C:210:PRO:HD3	2.01	0.42
2:H:17:ASN:HA	2:H:72:PRO:O	2.18	0.42
1:A:217:TRP:HB2	1:A:228:MET:HE2	2.01	0.42
1:A:14:ARG:HD3	1:A:20:PRO:HA	2.01	0.42
1:A:121:ARG:HH22	2:D:2:GLN:CB	2.28	0.42
1:E:234:ARG:HH11	2:F:8:GLN:HE21	1.67	0.42
1:E:74:PHE:CD2	1:E:95:LEU:HD23	2.54	0.42
1:E:119:GLU:O	2:F:1:ILE:HB	2.20	0.42
1:E:274:TRP:O	1:E:276:PRO:HD3	2.19	0.42
1:A:82:LEU:HD11	1:A:89:ALA:N	2.28	0.42
1:C:274:TRP:O	1:C:276:PRO:HD3	2.19	0.42
1:E:155[B]:HIS:CB	3:L:6:THR:HG21	2.49	0.42
1:E:218:GLN:NE2	1:E:221:GLY:HA2	2.35	0.42
1:A:121:ARG:HH22	2:D:2:GLN:H	1.67	0.42
2:H:23:LEU:O	2:H:67:HIS:HA	2.19	0.42
1:C:100:GLY:O	1:C:160:LEU:HD22	2.19	0.42
1:E:155[A]:HIS:HD2	3:L:6:THR:HG22	1.82	0.42
1:E:23:ILE:HD12	2:F:54:MET:SD	2.60	0.42
2:B:17:ASN:HD22	2:B:17:ASN:HA	1.71	0.41
1:E:203:CYS:HB2	1:E:217:TRP:CZ2	2.56	0.41
1:E:217:TRP:HB2	1:E:228:MET:HE2	2.02	0.41
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.85	0.41
1:A:194:ARG:HG3	1:A:198:GLU:O	2.20	0.41
1:E:81:LEU:HA	1:E:84:TYR:CD2	2.56	0.41
1:G:231:VAL:HB	2:H:8:GLN:HE22	1.85	0.41
2:H:79:ALA:HB2	2:H:94:TYR:CD1	2.55	0.41
1:A:107:TRP:CE3	1:E:269:PRO:HD3	2.56	0.41
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.55	0.41
1:G:28:VAL:HG23	1:G:33:PHE:CD1	2.56	0.41
2:F:31:HIS:CD2	2:F:32:PRO:HA	2.56	0.41
1:G:145:ARG:NH1	5:G:418:HOH:O	2.54	0.41
2:F:2:GLN:HB2	1:G:121:ARG:HH12	1.86	0.41
1:G:106:ASP:OD2	1:G:108:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.57	0.40
2:D:4:THR:HA	2:D:5:PRO:HD3	1.89	0.40
1:G:48:ARG:NH2	2:H:53:ASP:OD2	2.53	0.40
2:H:64:ILE:CD1	2:H:64:ILE:CB	2.84	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	278/281 (99%)	255 (92%)	21 (8%)	2 (1%)	22	59
1	C	277/281 (99%)	255 (92%)	19 (7%)	3 (1%)	14	48
1	E	277/281 (99%)	260 (94%)	14 (5%)	3 (1%)	14	48
1	G	276/281 (98%)	257 (93%)	16 (6%)	3 (1%)	14	48
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
2	D	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
2	F	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	H	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	K	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1528/1560 (98%)	1423 (93%)	94 (6%)	11 (1%)	22	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	SER
1	E	88	SER
1	E	89	ALA
1	A	88	SER
1	G	220	ASN
1	A	253	LYS
1	C	253	LYS
1	G	226	GLN
1	C	251	LEU
1	E	253	LYS
1	G	253	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/239 (100%)	203 (85%)	35 (15%)	3	13
1	C	237/239 (99%)	206 (87%)	31 (13%)	4	18
1	E	237/239 (99%)	201 (85%)	36 (15%)	3	12
1	G	236/239 (99%)	204 (86%)	32 (14%)	3	16
2	B	94/94 (100%)	86 (92%)	8 (8%)	10	36
2	D	94/94 (100%)	87 (93%)	7 (7%)	13	43
2	F	94/94 (100%)	87 (93%)	7 (7%)	13	43
2	H	94/94 (100%)	90 (96%)	4 (4%)	29	62
3	I	8/8 (100%)	8 (100%)	0	100	100
3	J	8/8 (100%)	8 (100%)	0	100	100
3	K	8/8 (100%)	8 (100%)	0	100	100
3	L	8/8 (100%)	7 (88%)	1 (12%)	4	19
All	All	1356/1364 (99%)	1195 (88%)	161 (12%)	5	21

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	14	ARG
1	A	18	GLU
1	A	19	GLU
1	A	39	ASP
1	A	41	GLU
1	A	44	ARG
1	A	46	GLU
1	A	65	GLN
1	A	81	LEU
1	A	82	LEU
1	A	88	SER
1	A	94	THR
1	A	121	ARG
1	A	122	ASP
1	A	130	LEU
1	A	141	GLN
1	A	149	GLN
1	A	163	GLU
1	A	179	LEU
1	A	184	SER
1	A	194	ARG
1	A	200	THR
1	A	214	THR
1	A	222	GLU
1	A	227	ASP
1	A	247	VAL
1	A	249	VAL
1	A	251	LEU
1	A	254	GLU
1	A	256	ASN
1	A	258	THR
1	A	260	ARG
1	A	266	LEU
1	A	273	ARG
2	B	0	MET
2	B	19	LYS
2	B	36	GLU
2	B	40	LEU
2	B	51	MET
2	B	64	ILE
2	B	73	THR
2	B	99	MET

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Mol	Chain	Res	Type
1	C	13	SER
1	C	18	GLU
1	C	39	ASP
1	C	41	GLU
1	C	46	GLU
1	C	65	GLN
1	C	82	LEU
1	C	94	THR
1	C	121	ARG
1	C	122	ASP
1	C	130	LEU
1	C	141	GLN
1	C	163	GLU
1	C	179	LEU
1	C	181	ARG
1	C	184	SER
1	C	194	ARG
1	C	214	THR
1	C	222	GLU
1	C	223	GLU
1	C	225	THR
1	C	227	ASP
1	C	230	LEU
1	C	251	LEU
1	C	254	GLU
1	C	256	ASN
1	C	258	THR
1	C	260	ARG
1	C	266	LEU
1	C	272	LEU
1	C	275	GLU
2	D	0	MET
2	D	36	GLU
2	D	40	LEU
2	D	61	SER
2	D	64	ILE
2	D	68	THR
2	D	73	THR
1	E	12	VAL
1	E	18	GLU
1	E	19	GLU
1	E	39	ASP

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Mol	Chain	Res	Type
1	E	41	GLU
1	E	44	ARG
1	E	46	GLU
1	E	61	GLU
1	E	65	GLN
1	E	81	LEU
1	E	82	LEU
1	E	92	SER
1	E	94	THR
1	E	96	GLN
1	E	111	ARG
1	E	122	ASP
1	E	130	LEU
1	E	163	GLU
1	E	173	LYS
1	E	179	LEU
1	E	181	ARG
1	E	184	SER
1	E	194	ARG
1	E	214	THR
1	E	224	LEU
1	E	226	GLN
1	E	230	LEU
1	E	251	LEU
1	E	254	GLU
1	E	256	ASN
1	E	258	THR
1	E	260	ARG
1	E	266	LEU
1	E	272	LEU
1	E	273	ARG
1	E	275	GLU
2	F	0	MET
2	F	19	LYS
2	F	36	GLU
2	F	40	LEU
2	F	51	MET
2	F	64	ILE
2	F	73	THR
1	G	13	SER
1	G	18	GLU
1	G	39	ASP

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Mol	Chain	Res	Type
1	G	41	GLU
1	G	44	ARG
1	G	46	GLU
1	G	65	GLN
1	G	79	ARG
1	G	82	LEU
1	G	94	THR
1	G	122	ASP
1	G	130	LEU
1	G	141	GLN
1	G	145	ARG
1	G	163	GLU
1	G	173	LYS
1	G	179	LEU
1	G	184	SER
1	G	194	ARG
1	G	214	THR
1	G	226	GLN
1	G	230	LEU
1	G	231	VAL
1	G	249	VAL
1	G	251	LEU
1	G	254	GLU
1	G	256	ASN
1	G	258	THR
1	G	260	ARG
1	G	266	LEU
1	G	272	LEU
1	G	275	GLU
2	H	0	MET
2	H	36	GLU
2	H	64	ILE
2	H	73	THR
3	L	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	169	HIS
1	A	188	HIS
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	255	GLN
1	A	256	ASN
1	A	263	HIS
2	B	8	GLN
2	B	17	ASN
2	B	31	HIS
1	C	65	GLN
1	C	72	GLN
1	C	141	GLN
1	C	169	HIS
1	C	188	HIS
1	C	256	ASN
1	C	263	HIS
2	D	2	GLN
2	D	8	GLN
2	D	17	ASN
2	D	31	HIS
1	E	72	GLN
1	E	169	HIS
1	E	188	HIS
1	E	256	ASN
1	E	263	HIS
2	F	2	GLN
2	F	8	GLN
2	F	17	ASN
2	F	31	HIS
2	F	38	GLN
1	G	65	GLN
1	G	70	GLN
1	G	80	ASN
1	G	141	GLN
1	G	155	HIS
1	G	169	HIS
1	G	188	HIS
1	G	218	GLN
1	G	256	ASN
1	G	263	HIS
2	H	2	GLN
2	H	6	GLN
2	H	8	GLN
2	H	17	ASN

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Mol	Chain	Res	Type
2	H	31	HIS
3	J	3	ASN
3	J	5	ASN
3	L	3	ASN
3	L	5	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	SO4	C	301	-	4,4,4	0.16	0	6,6,6	0.26	0
4	SO4	E	301	-	4,4,4	0.28	0	6,6,6	0.27	0
4	SO4	A	301	-	4,4,4	0.39	0	6,6,6	0.44	0
4	SO4	A	302	-	4,4,4	0.21	0	6,6,6	0.24	0
4	SO4	G	301	-	4,4,4	0.20	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	277/281 (98%)	-0.30	0	100	100	18, 43, 83, 104	0
1	C	277/281 (98%)	-0.38	0	100	100	13, 38, 83, 108	2 (0%)
1	E	277/281 (98%)	-0.22	0	100	100	23, 47, 89, 102	1 (0%)
1	G	277/281 (98%)	-0.27	0	100	100	21, 44, 77, 95	0
2	B	100/100 (100%)	-0.26	2 (2%)	65	50	19, 39, 61, 106	1 (1%)
2	D	100/100 (100%)	-0.33	1 (1%)	82	73	18, 39, 66, 101	1 (1%)
2	F	100/100 (100%)	-0.02	3 (3%)	50	33	25, 51, 79, 113	1 (1%)
2	H	100/100 (100%)	-0.27	2 (2%)	65	50	21, 38, 62, 101	1 (1%)
3	I	9/9 (100%)	-0.32	0	100	100	31, 38, 49, 53	0
3	J	9/9 (100%)	-0.59	0	100	100	20, 29, 40, 43	0
3	K	9/9 (100%)	-0.15	0	100	100	23, 38, 47, 54	0
3	L	9/9 (100%)	-0.02	0	100	100	42, 47, 59, 59	0
All	All	1544/1560 (98%)	-0.28	8 (0%)	91	86	13, 42, 83, 113	7 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	0	MET	5.4
2	D	0	MET	4.4
2	F	2	GLN	3.9
2	B	0	MET	3.8
2	H	0	MET	3.7
2	F	1	ILE	3.2
2	H	1	ILE	3.1
2	B	1	ILE	2.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	301	5/5	0.95	0.19	98,98,99,99	0
4	SO4	G	301	5/5	0.96	0.23	84,86,87,88	0
4	SO4	A	301	5/5	0.97	0.16	46,47,49,53	0
4	SO4	A	302	5/5	0.97	0.18	75,76,76,77	0
4	SO4	E	301	5/5	0.98	0.10	53,54,55,58	0

6.5 Other polymers (i)

There are no such residues in this entry.