Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2026 – 02:16 PM JST

PDB ID	:	44JE / pdb_000044je
Title	:	KIR2DS2 bound to HLA-C*07:02 presenting the RL9 peptide
Authors	:	Faoro, C.; Rossjohn, J.; Pymm, P.
Deposited on	:	2026-07-31
Resolution	:	2.90 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:

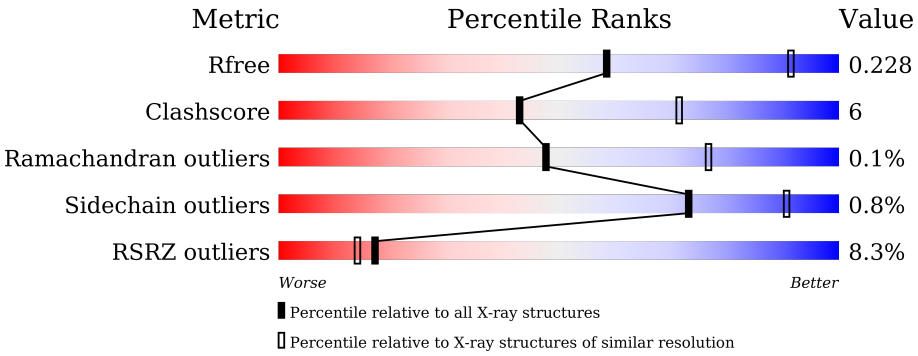
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	284	3% 82% 15% ·
1	E	284	2% 85% 13% ·
1	I	284	3% 82% 17% ·
1	N	284	19% 83% 13% ·
2	B	100	2% 93% 7%
2	F	100	3% 90% 10%

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Mol	Chain	Length	Quality of chain
2	L	100	2% 75% 25%
2	O	100	41% 76% 23%
3	C	9	89% 11%
3	G	9	89% 11%
3	M	9	11% 67% 33%
3	P	9	11% 89% 11%
4	D	202	5% 91% 7%
4	H	202	10% 81% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15524 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 HLA class I histocompatibility antigen, C alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2252	1391	417	437	7			
1	E	277	Total	C	N	O	S	0	0	0
			2222	1375	407	433	7			
1	I	281	Total	C	N	O	S	0	0	0
			2248	1391	410	440	7			
1	N	275	Total	C	N	O	S	0	0	0
			2156	1336	395	418	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			829	528	140	157	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			829	528	140	157	4			
2	O	100	Total	C	N	O	S	0	0	0
			800	512	135	149	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769

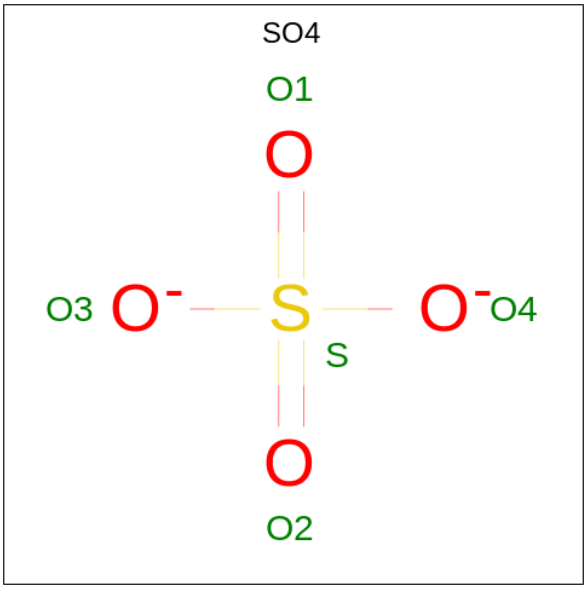
- Molecule 3 is a protein called Peptide RL9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			73	46	15	12			
3	G	9	Total	C	N	O	0	0	0
			73	46	15	12			
3	M	9	Total	C	N	O	0	0	0
			73	46	15	12			
3	P	9	Total	C	N	O	0	0	0
			73	46	15	12			

- Molecule 4 is a protein called Killer cell immunoglobulin-like receptor 2DS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1519	958	263	291	7			
4	H	194	Total	C	N	O	S	0	2	0
			1520	958	269	286	7			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

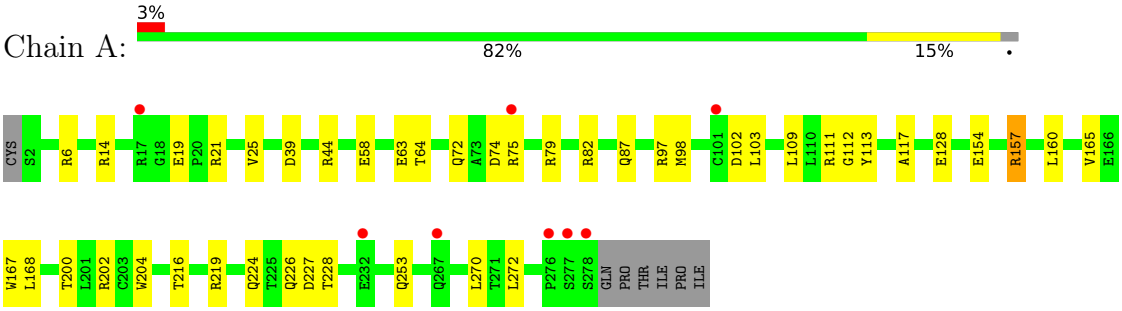


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	S		0	0
			5	4	1			
5	A	1	Total	O	S		0	0
			5	4	1			
5	D	1	Total	O	S		0	0
			5	4	1			
5	E	1	Total	O	S		0	0
			5	4	1			

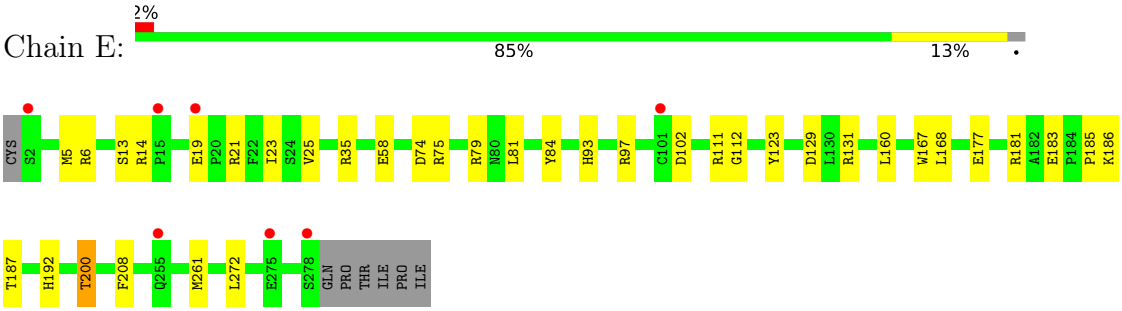
3 Residue-property plots (i)

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.

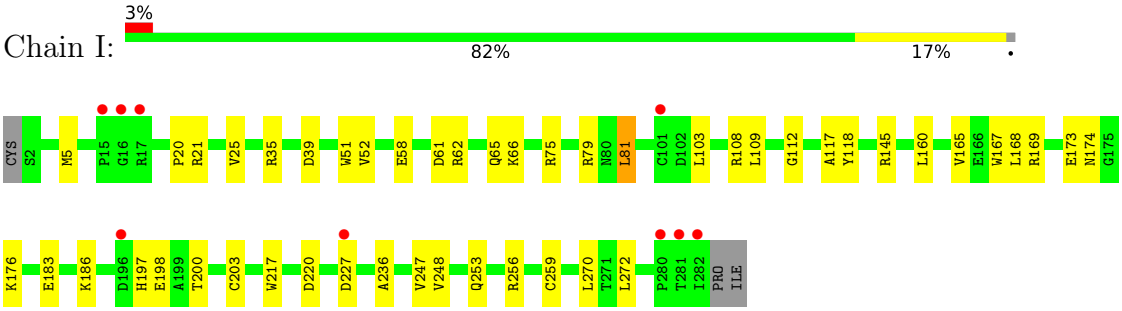
• Molecule 1: HLA class I histocompatibility antigen, C alpha chain



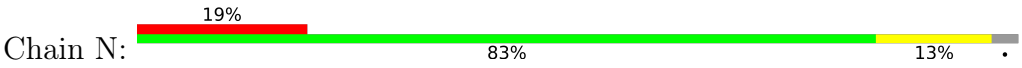
• Molecule 1: HLA class I histocompatibility antigen, C alpha chain

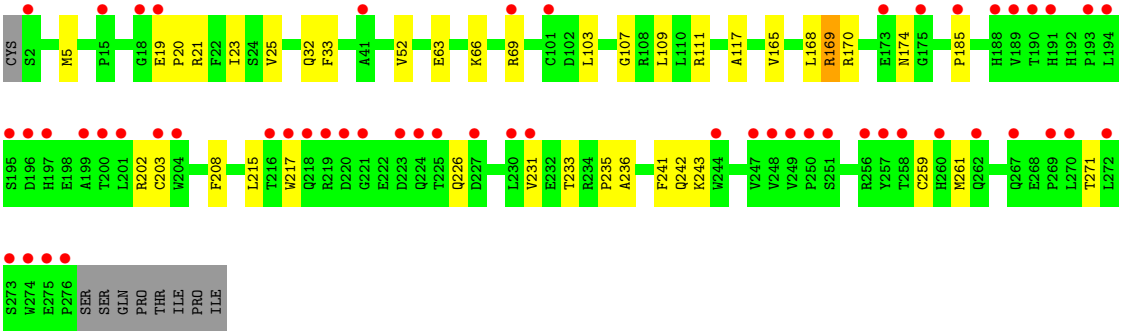


• Molecule 1: HLA class I histocompatibility antigen, C alpha chain

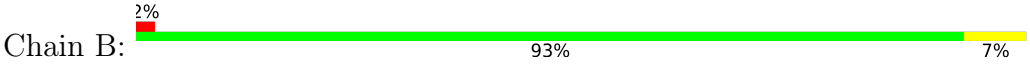


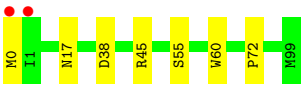
• Molecule 1: HLA class I histocompatibility antigen, C alpha chain



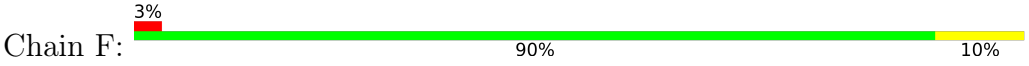


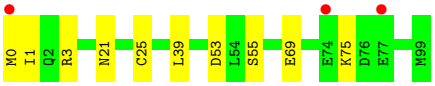
• Molecule 2: Beta-2-microglobulin





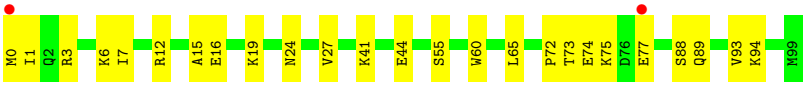
• Molecule 2: Beta-2-microglobulin



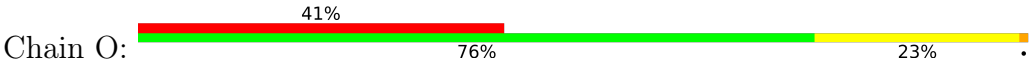


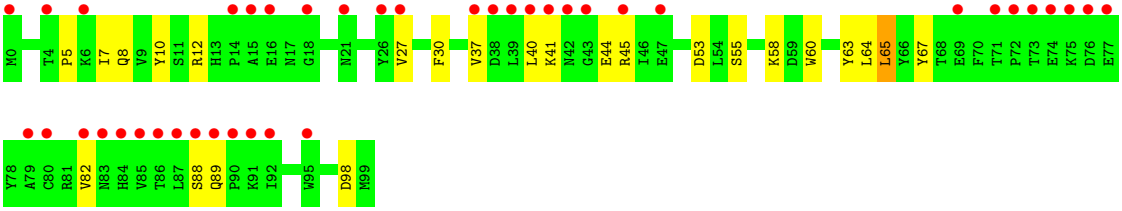
• Molecule 2: Beta-2-microglobulin



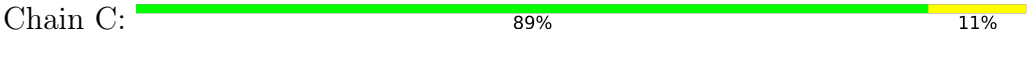


• Molecule 2: Beta-2-microglobulin





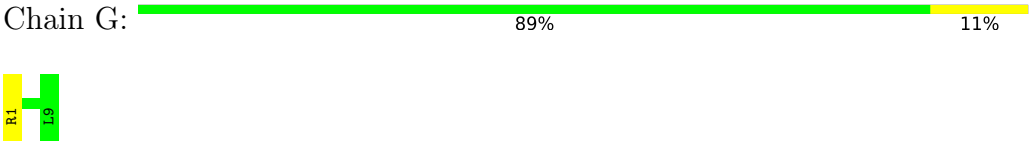
• Molecule 3: Peptide RL9





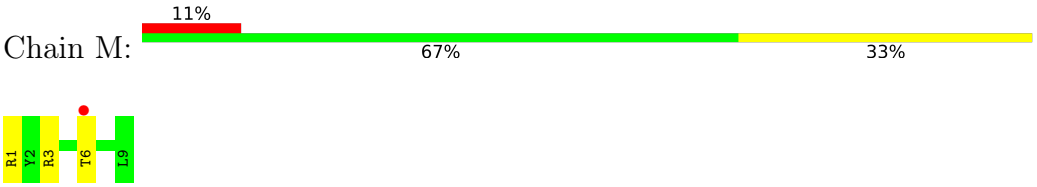
• Molecule 3: Peptide RL9

Chain G:



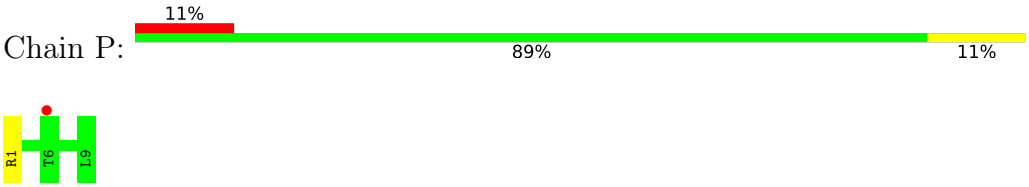
• Molecule 3: Peptide RL9

Chain M:



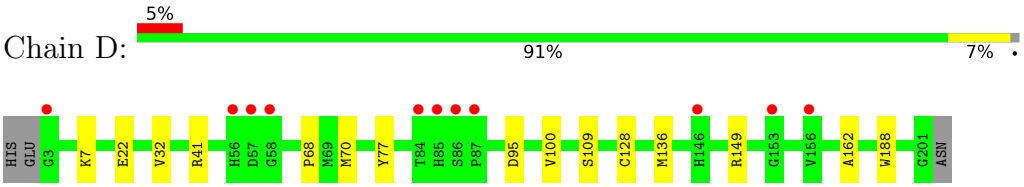
• Molecule 3: Peptide RL9

Chain P:



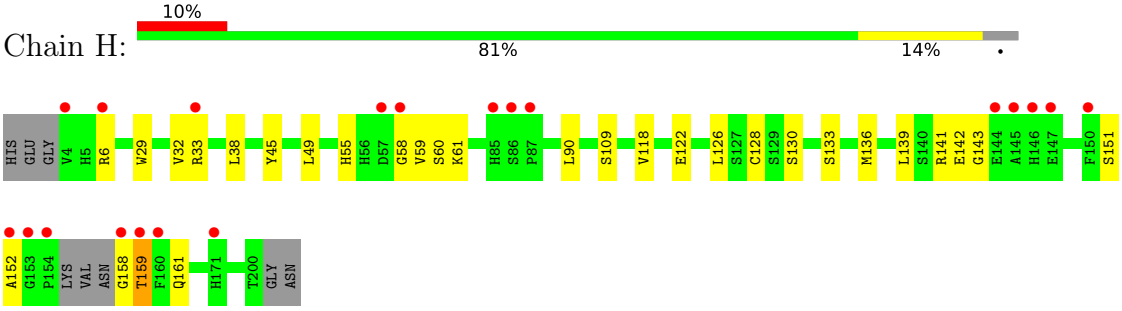
• Molecule 4: Killer cell immunoglobulin-like receptor 2DS2

Chain D:



• Molecule 4: Killer cell immunoglobulin-like receptor 2DS2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.64Å 116.99Å 144.76Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	73.98 – 2.90 73.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (73.98-2.90) 99.9 (73.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.195 , 0.230 0.196 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15524	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.19	0/2309	0.37	0/3133
1	E	0.16	0/2279	0.35	0/3095
1	I	0.16	0/2306	0.37	0/3134
1	N	0.16	0/2211	0.39	0/3007
2	B	0.15	0/852	0.40	0/1153
2	F	0.14	0/860	0.38	0/1162
2	L	0.17	0/852	0.38	0/1153
2	O	0.17	0/823	0.39	0/1117
3	C	0.10	0/74	0.34	0/98
3	G	0.15	0/74	0.27	0/98
3	M	0.13	0/74	0.24	0/98
3	P	0.13	0/74	0.41	0/98
4	D	0.14	0/1565	0.36	0/2129
4	H	0.14	0/1565	0.35	0/2125
All	All	0.16	0/15918	0.37	0/21600

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	2252	0	2106	35	0
1	E	2222	0	2071	28	0
1	I	2248	0	2089	31	0
1	N	2156	0	1975	34	0
2	B	829	0	788	5	0
2	F	837	0	803	7	0
2	L	829	0	788	18	0
2	O	800	0	729	18	0
3	C	73	0	79	2	0
3	G	73	0	79	2	0
3	M	73	0	79	2	0
3	P	73	0	79	1	0
4	D	1519	0	1428	9	0
4	H	1520	0	1440	19	0
5	A	10	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
All	All	15524	0	14533	185	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 6.

All (185) 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:O:88:SER:OG	2:O:89:GLN:OE1	1.97	0.82
1:N:202:ARG:NH1	2:O:98:ASP:O	2.20	0.75
1:N:107:GLY:O	1:N:169:ARG:NH1	2.21	0.74
1:E:79:ARG:NH1	1:E:79:ARG:O	2.21	0.73
1:N:235:PRO:HA	1:N:241:PHE:HD2	1.54	0.72
1:I:183:GLU:OE2	1:I:186:LYS:NZ	2.25	0.69
1:N:170:ARG:HH21	1:N:174:ASN:HD21	1.37	0.69
4:H:33[B]:ARG:NH1	4:H:58:GLY:O	2.26	0.68
1:A:226:GLN:H	1:A:226:GLN:CD	2.04	0.65
2:L:1:ILE:HD12	2:L:3:ARG:HH11	1.62	0.65
1:N:235:PRO:HG2	2:O:65:LEU:HD13	1.80	0.64
1:N:66:LYS:HG2	1:N:69:ARG:NH2	2.14	0.63
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.79	0.63
1:A:111:ARG:HG3	1:A:111:ARG:HH11	1.64	0.63
4:H:118:VAL:HG13	4:H:122:GLU:HB2	1.81	0.62
2:L:88:SER:OG	2:L:89:GLN:OE1	2.17	0.62
1:E:186:LYS:HD2	1:E:186:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ARG:NH2	1:E:102:ASP:OD1	2.33	0.60
1:E:167:TRP:CE2	3:G:1:ARG:HD2	2.38	0.59
1:N:215:LEU:HG	1:N:261:MET:HE2	1.85	0.58
1:I:220:ASP:OD2	1:I:256:ARG:NH2	2.27	0.58
1:A:82:ARG:HG2	1:A:87:GLN:HB2	1.86	0.58
1:N:203:CYS:HB2	1:N:217:TRP:CZ2	2.39	0.58
1:E:111:ARG:NH1	1:E:112:GLY:O	2.37	0.57
2:O:63:TYR:O	2:O:64:LEU:HD23	2.04	0.57
2:L:7:ILE:HG12	2:L:27:VAL:HG12	1.87	0.57
1:A:58:GLU:OE2	2:L:0:MET:N	2.37	0.56
1:E:183:GLU:OE2	1:E:186:LYS:NZ	2.36	0.56
1:I:200:THR:HG22	1:I:248:VAL:HG22	1.87	0.56
4:H:133:SER:HB3	4:H:158:GLY:HA2	1.88	0.56
1:A:72:GLN:HG2	1:A:75[A]:ARG:NH1	2.21	0.56
2:O:37:VAL:HG22	2:O:82:VAL:HG22	1.87	0.56
1:I:109:LEU:HB2	1:I:165:VAL:HG21	1.89	0.55
1:N:21:ARG:HE	1:N:23:ILE:HD11	1.72	0.55
1:N:226:GLN:H	1:N:226:GLN:CD	2.13	0.54
1:N:5:MET:HB2	1:N:168:LEU:HD13	1.89	0.54
1:N:103:LEU:HG	1:N:168:LEU:HD23	1.89	0.54
4:D:149:ARG:HG2	4:D:162:ALA:HB1	1.89	0.54
1:N:32:GLN:NE2	2:O:53:ASP:OD2	2.39	0.54
1:I:197:HIS:ND1	1:I:198:GLU:HG3	2.23	0.54
1:E:75:ARG:HG2	4:H:45:TYR:CZ	2.43	0.53
4:H:151:SER:OG	4:H:152:ALA:N	2.41	0.53
4:D:7:LYS:NZ	4:D:95:ASP:OD1	2.41	0.53
1:I:103:LEU:HG	1:I:168:LEU:HD23	1.91	0.53
1:N:235:PRO:O	2:O:10:TYR:OH	2.22	0.53
1:A:79:ARG:NH1	1:A:79:ARG:O	2.41	0.53
2:L:73:THR:HB	2:L:75:LYS:HE3	1.90	0.52
1:E:167:TRP:CG	3:G:1:ARG:HG3	2.44	0.52
1:I:253:GLN:NE2	1:I:256:ARG:HH11	2.07	0.52
1:A:109:LEU:HB2	1:A:165:VAL:HG21	1.91	0.51
2:L:1:ILE:HD12	2:L:3:ARG:NH1	2.23	0.51
1:E:192:HIS:HB2	1:E:200:THR:HG23	1.91	0.51
1:E:5:MET:HB2	1:E:168:LEU:HD13	1.91	0.51
1:E:81:LEU:HD21	1:E:123:TYR:CZ	2.46	0.51
4:H:55:HIS:ND1	4:H:60:SER:OG	2.41	0.51
1:N:185:PRO:HB3	1:N:208:PHE:HD2	1.74	0.51
1:N:233:THR:OG1	1:N:243:LYS:HE2	2.11	0.51
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:GLU:H	1:E:58:GLU:CD	2.19	0.50
1:A:111:ARG:HG2	1:A:113:TYR:CZ	2.47	0.50
2:B:0:MET:SD	2:B:0:MET:N	2.72	0.50
4:H:128:CYS:O	4:H:161:GLN:HA	2.11	0.50
1:I:259:CYS:HB3	1:I:272:LEU:HB2	1.94	0.50
1:I:75:ARG:NH2	1:I:79:ARG:HG3	2.27	0.50
4:D:68:PRO:O	4:D:70:MET:HE2	2.12	0.50
1:E:21:ARG:HH21	1:E:23:ILE:HD11	1.77	0.49
1:E:185:PRO:HG2	1:E:261:MET:HE1	1.94	0.49
1:N:203:CYS:SG	1:N:261:MET:HE3	2.52	0.49
1:I:108:ARG:HA	1:I:169:ARG:HH21	1.78	0.49
1:N:109:LEU:HB2	1:N:165:VAL:HG21	1.95	0.49
2:O:41:LYS:O	2:O:44:GLU:HG2	2.13	0.49
4:D:100:VAL:HG11	4:D:188:TRP:CD2	2.47	0.49
1:E:25:VAL:HG21	2:F:55:SER:HB2	1.95	0.49
1:I:20:PRO:HD2	1:I:75:ARG:HG3	1.95	0.49
1:N:185:PRO:HB3	1:N:208:PHE:HB3	1.95	0.49
1:E:35:ARG:NH1	2:F:53:ASP:OD1	2.46	0.48
1:A:63:GLU:OE2	3:C:1:ARG:NH1	2.45	0.48
3:M:3:ARG:HH12	3:M:6:THR:HG22	1.78	0.48
2:O:65:LEU:HD23	2:O:67:TYR:HD2	1.77	0.48
1:N:208:PHE:CE1	1:N:241:PHE:HB2	2.48	0.48
4:H:29:TRP:CE3	4:H:59:VAL:HG21	2.48	0.48
1:N:63:GLU:OE2	3:P:1:ARG:HD2	2.13	0.48
1:E:185:PRO:HB3	1:E:208:PHE:HB3	1.95	0.47
4:H:33[B]:ARG:HH12	4:H:58:GLY:C	2.19	0.47
4:H:33[A]:ARG:HG3	4:H:55:HIS:CE1	2.50	0.47
1:N:165:VAL:O	1:N:169:ARG:HD3	2.15	0.47
1:I:174:ASN:N	1:I:174:ASN:HD22	2.11	0.47
1:A:154:GLU:HG2	1:A:157:ARG:NH2	2.29	0.47
1:N:25:VAL:HG21	2:O:55:SER:HB2	1.95	0.47
4:H:126:LEU:HD12	4:H:139:LEU:HD21	1.97	0.47
1:N:21:ARG:HH21	1:N:23:ILE:HD11	1.80	0.47
1:N:117:ALA:HB2	2:O:60:TRP:CE2	2.50	0.47
1:A:111:ARG:NH1	1:A:128:GLU:HA	2.30	0.47
1:E:13:SER:HB2	1:E:93:HIS:H	1.78	0.47
2:O:5:PRO:HB3	2:O:30:PHE:HB3	1.97	0.47
2:F:21:ASN:O	2:F:69:GLU:HG3	2.15	0.46
4:H:109:SER:O	4:H:128:CYS:HA	2.14	0.46
2:B:38:ASP:OD2	2:B:45:ARG:HD2	2.15	0.46
1:E:177:GLU:O	1:E:181:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLN:O	1:A:228:THR:OG1	2.20	0.46
4:H:29:TRP:HE3	4:H:59:VAL:HG21	1.80	0.46
2:O:7:ILE:HG12	2:O:27:VAL:HG12	1.97	0.46
1:E:112:GLY:HA3	1:E:160:LEU:HD13	1.98	0.46
1:A:226:GLN:OE1	1:A:226:GLN:N	2.38	0.46
2:O:40:LEU:HD23	2:O:45:ARG:HA	1.98	0.46
4:H:38:LEU:HD22	4:H:90:LEU:HD21	1.98	0.45
1:I:25:VAL:HG21	2:L:55:SER:HB2	1.99	0.45
1:I:203:CYS:HB2	1:I:217:TRP:CZ2	2.52	0.45
4:D:22:GLU:HB3	1:I:145:ARG:HH12	1.82	0.45
2:F:75:LYS:HD3	2:F:75:LYS:H	1.81	0.45
1:I:58:GLU:H	1:I:58:GLU:CD	2.24	0.45
1:I:253:GLN:HE22	1:I:256:ARG:HH11	1.64	0.45
1:A:111:ARG:HG2	1:A:113:TYR:CE1	2.52	0.45
1:E:74:ASP:OD1	1:E:97:ARG:NH2	2.42	0.45
1:A:167:TRP:CD2	3:C:1:ARG:HG3	2.52	0.45
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.98	0.45
1:A:25:VAL:HG21	2:B:55:SER:HB2	1.97	0.44
4:H:130:SER:O	4:H:159:THR:HA	2.16	0.44
2:L:41:LYS:O	2:L:44:GLU:HG2	2.17	0.44
1:A:219:ARG:HH12	1:A:253:GLN:HE22	1.63	0.44
1:I:173:GLU:O	1:I:176:LYS:HB2	2.17	0.44
2:L:6:LYS:O	2:L:27:VAL:HA	2.17	0.44
1:N:170:ARG:HH21	1:N:174:ASN:ND2	2.09	0.44
1:A:226:GLN:HG2	1:A:227:ASP:OD2	2.18	0.44
1:I:62:ARG:HA	1:I:62:ARG:HD2	1.86	0.44
1:A:74:ASP:OD1	1:A:97:ARG:NH2	2.43	0.44
1:I:21:ARG:HD2	1:I:39:ASP:OD1	2.17	0.44
4:D:136:MET:HG3	4:D:149:ARG:O	2.18	0.44
1:E:187:THR:HB	1:E:272:LEU:HD11	2.00	0.44
1:I:167:TRP:CG	3:M:1:ARG:HG3	2.53	0.44
1:I:61:ASP:O	1:I:65:GLN:HB2	2.18	0.44
1:A:14:ARG:NH2	1:A:19:GLU:O	2.43	0.43
1:A:72:GLN:HG2	1:A:75[A]:ARG:CZ	2.48	0.43
2:L:74:GLU:H	2:L:74:GLU:HG2	1.65	0.43
1:A:72:GLN:HA	1:A:75[B]:ARG:HB3	2.00	0.43
2:F:0:MET:HE3	2:F:0:MET:HB3	1.80	0.43
4:D:41:ARG:HD3	4:D:77:TYR:OH	2.19	0.43
1:I:5:MET:HB2	1:I:168:LEU:HD13	2.00	0.43
1:A:6:ARG:HD2	1:A:98:MET:SD	2.58	0.43
1:I:51:TRP:CE3	1:I:52:VAL:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:HA3	1:A:160:LEU:HD13	2.01	0.43
1:A:111:ARG:HH12	1:A:128:GLU:HA	1.84	0.43
1:N:242:GLN:NE2	2:O:12:ARG:O	2.51	0.43
1:E:81:LEU:HD23	1:E:84:TYR:CD2	2.53	0.43
1:I:236:ALA:O	2:L:12:ARG:HG3	2.18	0.43
2:L:19:LYS:O	2:L:72:PRO:HD2	2.18	0.43
2:L:24:ASN:HB3	2:L:65:LEU:HD11	2.02	0.42
1:E:81:LEU:HD23	1:E:81:LEU:HA	1.71	0.42
1:I:117:ALA:HB2	2:L:60:TRP:CE2	2.54	0.42
1:E:261:MET:HE3	1:E:261:MET:HB3	1.81	0.42
1:I:112:GLY:HA3	1:I:160:LEU:HD13	2.01	0.42
1:N:19:GLU:HG3	1:N:20:PRO:HD2	2.01	0.42
1:N:111:ARG:HH11	1:N:111:ARG:HG2	1.83	0.42
1:A:74:ASP:CG	1:A:97:ARG:HH22	2.26	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.42
1:E:14:ARG:NH2	1:E:19:GLU:O	2.45	0.42
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.35	0.42
1:A:111:ARG:HG3	1:A:111:ARG:NH1	2.32	0.42
2:F:1:ILE:HD11	2:F:3:ARG:NH2	2.34	0.42
4:H:136:MET:HB2	4:H:136:MET:HE3	1.61	0.42
1:I:81:LEU:HD12	1:I:118:TYR:CG	2.55	0.42
1:N:236:ALA:O	2:O:12:ARG:HG3	2.19	0.42
4:H:118:VAL:CG1	4:H:122:GLU:HB2	2.50	0.41
2:L:15:ALA:O	2:L:16:GLU:HG3	2.20	0.41
1:A:21:ARG:HD2	1:A:39:ASP:OD2	2.20	0.41
1:N:235:PRO:HG2	2:O:65:LEU:CD1	2.49	0.41
1:A:219:ARG:HH12	1:A:253:GLN:NE2	2.17	0.41
1:E:79:ARG:HA	1:E:79:ARG:HD2	1.87	0.41
4:D:41:ARG:HD3	4:D:77:TYR:CZ	2.56	0.41
1:A:44:ARG:HG3	1:A:64:THR:OG1	2.21	0.41
1:N:231:VAL:HB	2:O:8:GLN:HE22	1.85	0.41
1:E:129:ASP:O	1:E:131:ARG:HG3	2.21	0.41
4:H:59:VAL:CG1	4:H:61:LYS:HE3	2.51	0.41
1:N:259:CYS:O	1:N:271:THR:HA	2.20	0.41
2:L:7:ILE:HG21	2:L:93:VAL:HG21	2.01	0.41
2:B:17:ASN:HA	2:B:72:PRO:O	2.20	0.40
1:I:227:ASP:O	1:I:247:VAL:HG23	2.21	0.40
4:H:141:ARG:O	4:H:143:GLY:N	2.55	0.40
1:A:270:LEU:HD23	1:A:272:LEU:HD11	2.03	0.40
4:D:109:SER:O	4:D:128:CYS:HA	2.21	0.40
1:I:62:ARG:HE	1:I:66:LYS:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:LEU:HD23	1:I:270:LEU:HA	1.94	0.40
2:L:73:THR:OG1	2:L:75:LYS:HG2	2.21	0.40
2:L:77:GLU:OE2	2:L:94:LYS:HB3	2.22	0.40
1:N:33:PHE:CD2	1:N:52:VAL:HG21	2.56	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	277/284 (98%)	270 (98%)	7 (2%)	0	100	100
1	E	275/284 (97%)	268 (98%)	7 (2%)	0	100	100
1	I	279/284 (98%)	270 (97%)	9 (3%)	0	100	100
1	N	273/284 (96%)	264 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	L	98/100 (98%)	98 (100%)	0	0	100	100
2	O	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	G	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
4	D	197/202 (98%)	192 (98%)	5 (2%)	0	100	100
4	H	192/202 (95%)	184 (96%)	6 (3%)	2 (1%)	12	39
All	All	1913/1976 (97%)	1865 (98%)	46 (2%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	142	GLU
4	H	159	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	233/240 (97%)	230 (99%)	3 (1%)	61 86
1	E	229/240 (95%)	228 (100%)	1 (0%)	84 94
1	I	232/240 (97%)	230 (99%)	2 (1%)	70 90
1	N	214/240 (89%)	213 (100%)	1 (0%)	81 93
2	B	93/95 (98%)	93 (100%)	0	100 100
2	F	95/95 (100%)	95 (100%)	0	100 100
2	L	93/95 (98%)	93 (100%)	0	100 100
2	O	84/95 (88%)	82 (98%)	2 (2%)	43 75
3	C	7/7 (100%)	7 (100%)	0	100 100
3	G	7/7 (100%)	7 (100%)	0	100 100
3	M	7/7 (100%)	7 (100%)	0	100 100
3	P	7/7 (100%)	7 (100%)	0	100 100
4	D	165/173 (95%)	164 (99%)	1 (1%)	78 93
4	H	166/173 (96%)	162 (98%)	4 (2%)	43 75
All	All	1632/1714 (95%)	1618 (99%)	14 (1%)	73 90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ARG
1	A	200	THR
1	A	216	THR
4	D	32	VAL
1	E	200	THR
4	H	6[A]	ARG

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Mol	Chain	Res	Type
4	H	6[B]	ARG
4	H	32	VAL
4	H	49	LEU
1	I	35	ARG
1	I	81	LEU
1	N	169	ARG
2	O	58	LYS
2	O	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	HIS
1	A	253	GLN
2	B	2	GLN
2	B	13	HIS
2	B	17	ASN
1	E	32	GLN
1	E	96	GLN
1	E	155	GLN
1	E	191	HIS
1	E	262	GLN
4	H	63	ASN
4	H	190	ASN
1	I	87	GLN
1	I	224	GLN
1	I	253	GLN
1	I	262	GLN
2	L	13	HIS
1	N	65	GLN
1	N	87	GLN
1	N	174	ASN
1	N	180	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
5	SO4	E	301	-	4,4,4	0.60	0	6,6,6	0.06	0
5	SO4	A	302	-	4,4,4	0.61	0	6,6,6	0.11	0
5	SO4	D	301	-	4,4,4	0.61	0	6,6,6	0.07	0
5	SO4	A	301	-	4,4,4	0.61	0	6,6,6	0.06	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

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	277/284 (97%)	-0.05	8 (2%) 53 45	23, 46, 78, 100	2 (0%)
1	E	277/284 (97%)	-0.09	7 (2%) 58 48	29, 45, 79, 111	0
1	I	281/284 (98%)	0.18	9 (3%) 50 41	27, 60, 93, 120	0
1	N	275/284 (96%)	0.91	55 (20%) 3 2	33, 74, 143, 157	0
2	B	100/100 (100%)	0.06	2 (2%) 65 56	34, 58, 83, 95	0
2	F	100/100 (100%)	0.04	3 (3%) 52 43	36, 56, 85, 103	0
2	L	100/100 (100%)	0.29	2 (2%) 65 56	38, 67, 108, 126	0
2	O	100/100 (100%)	1.75	41 (41%) 0 0	59, 110, 141, 152	0
3	C	9/9 (100%)	-0.25	0 100 100	37, 42, 51, 54	0
3	G	9/9 (100%)	-0.22	0 100 100	31, 41, 49, 55	0
3	M	9/9 (100%)	0.19	1 (11%) 10 9	43, 53, 68, 73	0
3	P	9/9 (100%)	0.25	1 (11%) 10 9	47, 54, 70, 79	0
4	D	199/202 (98%)	-0.04	11 (5%) 30 24	29, 45, 84, 117	0
4	H	194/202 (96%)	0.16	20 (10%) 12 10	28, 45, 101, 129	2 (1%)
All	All	1939/1976 (98%)	0.26	160 (8%) 17 14	23, 53, 119, 157	4 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	159	THR	5.7
1	N	196	ASP	5.3
4	D	57	ASP	5.3
1	N	257	TYR	5.2
4	H	158	GLY	4.9
1	N	185	PRO	4.6
4	H	58	GLY	4.5
4	D	56	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	N	220	ASP	4.4
2	O	86	THR	4.4
1	N	194	LEU	4.1
4	H	154	PRO	4.1
2	O	15	ALA	4.1
1	N	276	PRO	4.0
4	H	152	ALA	3.9
1	N	189	VAL	3.9
1	N	260	HIS	3.9
4	H	86	SER	3.9
2	O	45	ARG	3.8
1	N	223	ASP	3.8
2	O	95	TRP	3.8
2	O	73	THR	3.8
1	N	195	SER	3.7
2	B	0	MET	3.6
4	H	6[A]	ARG	3.6
1	N	227	ASP	3.6
2	L	0	MET	3.6
1	N	224	GLN	3.6
1	N	249	VAL	3.6
2	O	92	ILE	3.6
4	H	144	GLU	3.6
4	H	150	PHE	3.5
1	E	101	CYS	3.4
2	O	16	GLU	3.4
1	N	193	PRO	3.4
4	H	145	ALA	3.4
4	D	85	HIS	3.4
1	N	225	THR	3.4
1	A	101	CYS	3.3
4	H	85	HIS	3.3
2	O	71	THR	3.3
1	A	278	SER	3.3
1	E	278	SER	3.3
2	O	47	GLU	3.3
2	O	75	LYS	3.3
4	H	87	PRO	3.3
1	I	282	ILE	3.3
1	E	2	SER	3.3
1	A	232	GLU	3.2
2	O	74	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	281	THR	3.2
1	N	15	PRO	3.2
2	O	39	LEU	3.2
1	N	270	LEU	3.2
1	N	273	SER	3.1
1	N	197	HIS	3.1
4	H	160	PHE	3.1
4	H	4	VAL	3.1
2	O	90	PRO	3.1
1	N	201	LEU	3.1
2	O	91	LYS	3.1
1	N	41	ALA	3.1
1	N	272	LEU	3.1
2	O	85	VAL	3.1
4	D	153	GLY	3.0
1	N	230	LEU	3.0
1	N	250	PRO	3.0
1	A	277	SER	3.0
1	N	217	TRP	3.0
2	O	80	CYS	2.9
2	O	89	GLN	2.9
1	I	280	PRO	2.9
1	N	274	TRP	2.8
1	N	19	GLU	2.8
2	O	83	ASN	2.8
1	E	255	GLN	2.8
1	E	275	GLU	2.8
4	H	171	HIS	2.8
1	N	173	GLU	2.8
2	F	77	GLU	2.8
2	O	82	VAL	2.7
4	H	57	ASP	2.7
1	A	17	ARG	2.7
1	N	188	HIS	2.7
1	N	269	PRO	2.7
2	O	88	SER	2.7
4	H	146	HIS	2.7
3	P	6	THR	2.7
2	O	21	ASN	2.6
2	O	43	GLY	2.6
1	N	258	THR	2.6
1	N	199	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	4	THR	2.6
2	O	42	ASN	2.6
1	N	204	TRP	2.5
4	D	87	PRO	2.5
2	O	77	GLU	2.5
1	N	248	VAL	2.5
4	H	147	GLU	2.5
1	N	219	ARG	2.5
2	O	38	ASP	2.5
2	O	72	PRO	2.5
1	N	200	THR	2.5
2	O	79	ALA	2.5
1	A	276	PRO	2.4
1	N	256	ARG	2.4
2	L	77	GLU	2.4
1	N	262	GLN	2.4
2	O	0	MET	2.4
4	H	153	GLY	2.4
1	N	216	THR	2.4
3	M	6	THR	2.4
2	O	87	LEU	2.4
1	N	247	VAL	2.4
1	N	101	CYS	2.4
1	N	251	SER	2.4
2	B	1	ILE	2.4
4	D	58	GLY	2.3
4	D	84	THR	2.3
2	O	14	PRO	2.3
2	O	41	LYS	2.3
1	N	221	GLY	2.3
1	I	196	ASP	2.3
2	O	84	HIS	2.3
4	H	33[A]	ARG	2.3
4	D	3	GLY	2.3
1	N	190	THR	2.3
2	O	26	TYR	2.2
1	E	19	GLU	2.2
2	F	74	GLU	2.2
2	O	40	LEU	2.2
1	I	17	ARG	2.2
1	N	191	HIS	2.2
2	O	6	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	37	VAL	2.2
1	N	18	GLY	2.2
2	O	27	VAL	2.2
1	I	15	PRO	2.1
2	F	0	MET	2.1
1	A	75[A]	ARG	2.1
1	N	69	ARG	2.1
1	N	231	VAL	2.1
4	D	156	VAL	2.1
1	I	227	ASP	2.1
2	O	76	ASP	2.1
1	N	275	GLU	2.1
2	O	69	GLU	2.1
4	D	86	SER	2.1
1	N	218	GLN	2.1
1	N	267	GLN	2.1
2	O	18	GLY	2.1
1	N	2	SER	2.1
1	A	267	GLN	2.1
1	I	101	CYS	2.0
1	N	203	CYS	2.0
4	D	146	HIS	2.0
1	E	15	PRO	2.0
1	I	16	GLY	2.0
1	N	175	GLY	2.0
1	N	244	TRP	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 oligosaccharides 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
5	SO4	A	302	5/5	0.82	0.27	78,85,109,130	0
5	SO4	A	301	5/5	0.83	0.16	75,92,104,115	0
5	SO4	E	301	5/5	0.86	0.13	81,82,93,109	0
5	SO4	D	301	5/5	0.87	0.18	80,80,91,119	0

6.5 Other polymers (i)

There are no such residues in this entry.