



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:53 PM UTC

PDB ID : 3HF1 / pdb_00003hf1
Title : Crystal structure of human p53R2
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Deposited on : 2009-05-10
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

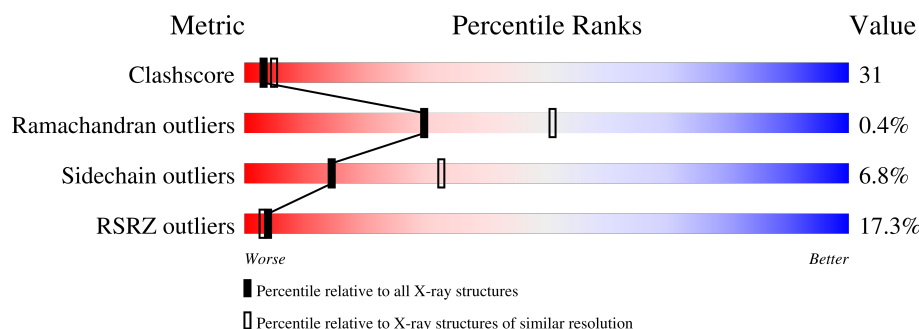
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	351	
1	B	351	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4718 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 Ribonucleoside-diphosphate reductase subunit M2 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2306	1509	376	410	11			
1	B	286	Total	C	N	O	S	0	0	0
			2354	1541	385	416	12			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	2	Total	Fe	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

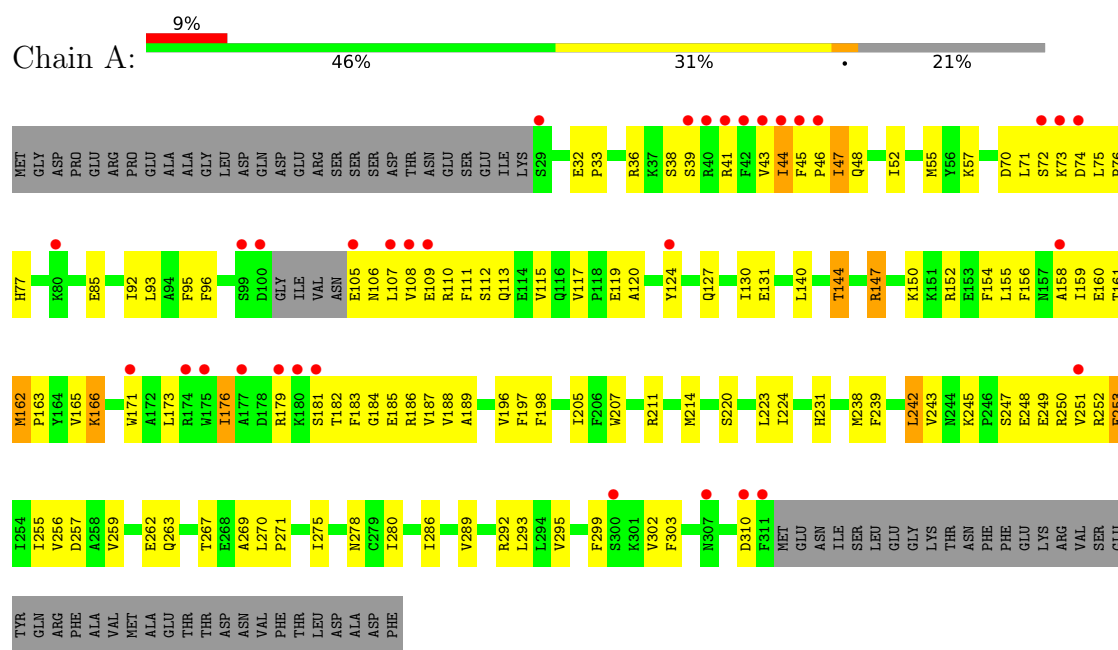
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	19	Total	O	0	0
			19	19		

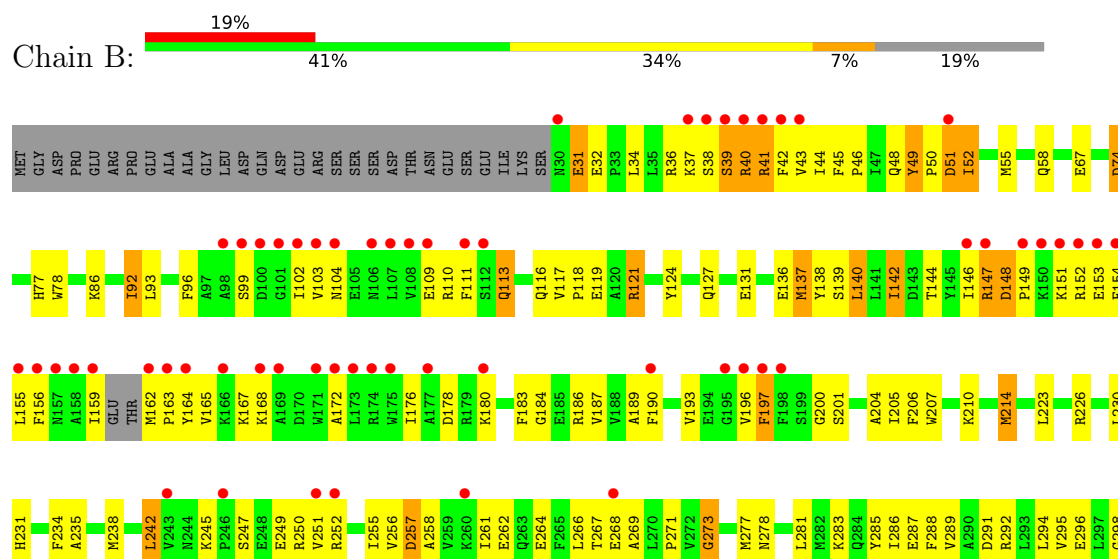
3 Residue-property plots [i](#)

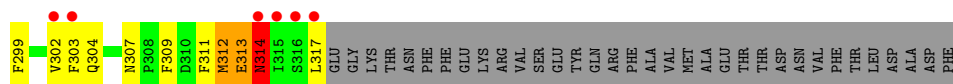
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribonucleoside-diphosphate reductase subunit M2 B



• Molecule 1: Ribonucleoside-diphosphate reductase subunit M2 B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.67Å 99.55Å 132.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	88.0 (50.00-2.60) 88.7 (50.00-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.273 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4718	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, FE

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	0.48	0/2366	1.01	13/3193 (0.4%)
1	B	0.44	0/2414	1.00	13/3257 (0.4%)
All	All	0.46	0/4780	1.01	26/6450 (0.4%)

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	B	0	2

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	162	MET	CA-C-N	9.19	128.52	118.97
1	A	162	MET	C-N-CA	9.19	128.52	118.97
1	A	196	VAL	CB-CA-C	-8.88	102.77	111.30
1	A	112	SER	N-CA-C	-8.43	103.00	113.20
1	A	162	MET	N-CA-C	7.69	118.97	110.13
1	B	147	ARG	N-CA-C	7.58	120.27	111.02
1	B	51	ASP	N-CA-C	7.54	119.14	111.07
1	B	50	PRO	N-CA-C	-7.42	104.58	113.86
1	A	154	PHE	N-CA-C	-6.56	104.21	111.82
1	B	38	SER	N-CA-C	-6.51	103.88	112.34
1	A	243	VAL	N-CA-C	-6.37	104.83	111.58
1	B	51	ASP	CB-CA-C	-6.35	100.91	110.88
1	B	273	GLY	N-CA-C	-6.12	106.76	114.16
1	B	257	ASP	N-CA-C	-6.07	105.72	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ASN	N-CA-C	5.94	118.92	109.65
1	B	142	ILE	CB-CA-C	-5.83	104.50	111.97
1	B	111	PHE	N-CA-C	5.83	118.41	111.71
1	B	52	ILE	N-CA-C	-5.69	104.80	111.00
1	A	47	ILE	N-CA-C	5.69	116.75	109.30
1	A	96	PHE	N-CA-C	-5.52	105.17	111.07
1	B	31	GLU	N-CA-C	-5.50	106.45	112.72
1	A	253	GLU	CB-CA-C	-5.41	102.38	110.88
1	A	253	GLU	N-CA-C	5.31	116.75	111.07
1	A	176	ILE	N-CA-C	5.31	116.58	112.12
1	A	211	ARG	N-CA-C	-5.25	106.65	113.16
1	B	74	ASP	N-CA-C	5.13	117.66	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	39	SER	Peptide
1	B	41	ARG	Peptide

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	2306	0	2282	149	0
1	B	2354	0	2338	165	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	26	0	0	3	0
4	B	19	0	0	0	0
All	All	4718	0	4620	290	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 31.

All (290) 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:B:153:GLU:OE1	1:B:154:PHE:HB2	1.46	1.16
1:B:148:ASP:HB2	1:B:149:PRO:CD	1.82	1.08
1:A:147:ARG:HD3	1:A:147:ARG:H	1.19	1.04
1:A:166:LYS:HE3	1:A:166:LYS:HA	1.38	1.03
1:A:107:LEU:HD21	1:A:127:GLN:HB3	1.42	1.02
1:B:146:ILE:HG21	1:B:151:LYS:HB3	1.39	1.00
1:A:43:VAL:HG13	1:A:44:ILE:H	1.25	1.00
1:A:44:ILE:HG22	1:B:139:SER:OG	1.65	0.97
1:A:44:ILE:HG23	1:A:45:PHE:H	1.32	0.94
1:B:184:GLY:HA2	1:B:242:LEU:HD21	1.50	0.94
1:B:153:GLU:OE1	1:B:154:PHE:CB	2.16	0.93
1:A:107:LEU:CD1	1:A:124:TYR:HD1	1.81	0.93
1:B:148:ASP:HB2	1:B:149:PRO:HD3	1.52	0.92
1:B:41:ARG:H	1:B:41:ARG:HD3	1.34	0.91
1:A:44:ILE:HG23	1:A:45:PHE:N	1.88	0.88
1:A:105:GLU:HB3	1:A:108:VAL:CG1	2.04	0.88
1:A:160:GLU:OE2	1:B:42:PHE:CE1	2.30	0.83
1:A:127:GLN:O	1:A:131:GLU:HG2	1.78	0.83
1:A:160:GLU:OE2	1:B:42:PHE:HE1	1.60	0.83
1:A:45:PHE:CE1	1:A:47:ILE:HD11	2.14	0.82
1:B:148:ASP:CB	1:B:149:PRO:CD	2.55	0.81
1:A:73:LYS:O	1:A:76:PRO:HD2	1.80	0.81
1:A:252:ARG:O	1:A:256:VAL:HG22	1.80	0.81
1:B:148:ASP:HB2	1:B:149:PRO:HD2	1.62	0.79
1:B:312:MET:HE2	1:B:312:MET:HA	1.65	0.79
1:B:153:GLU:OE1	1:B:154:PHE:CA	2.33	0.77
1:A:259:VAL:O	1:A:263:GLN:HG3	1.85	0.76
1:A:278:ASN:OD1	1:A:280:ILE:HG22	1.86	0.75
1:B:153:GLU:OE1	1:B:153:GLU:C	2.30	0.74
1:B:146:ILE:HG21	1:B:151:LYS:CB	2.17	0.73
1:B:238:MET:HA	1:B:238:MET:HE2	1.71	0.73
1:A:111:PHE:O	1:A:115:VAL:HG12	1.88	0.73
1:A:43:VAL:HG13	1:A:44:ILE:N	2.00	0.72
1:B:252:ARG:O	1:B:256:VAL:HG22	1.89	0.72
1:B:153:GLU:OE1	1:B:154:PHE:N	2.22	0.72
1:A:162:MET:O	1:A:165:VAL:HG12	1.90	0.71
1:B:40:ARG:CZ	1:B:48:GLN:HG2	2.20	0.71
1:A:71:LEU:HA	1:A:74:ASP:OD2	1.90	0.71
1:A:110:ARG:HH21	1:A:186:ARG:CD	2.03	0.71
1:A:140:LEU:O	1:A:144:THR:HG23	1.91	0.69
1:A:147:ARG:H	1:A:147:ARG:CD	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:HG23	1:B:234:PHE:HE1	1.57	0.69
1:B:189:ALA:O	1:B:193:VAL:HG23	1.93	0.69
1:A:107:LEU:CD1	1:A:124:TYR:CD1	2.72	0.69
1:B:137:MET:HE2	1:B:137:MET:HA	1.75	0.68
1:B:104:ASN:HD21	1:B:131:GLU:HG3	1.58	0.68
1:B:41:ARG:HD3	1:B:41:ARG:N	2.09	0.67
1:B:283:LYS:O	1:B:287:GLU:HG3	1.95	0.67
1:B:39:SER:HB2	1:B:116:GLN:HB3	1.76	0.66
1:B:77:HIS:HB3	1:B:214:MET:HE3	1.77	0.66
1:A:255:ILE:O	1:A:259:VAL:HG23	1.95	0.66
1:B:262:GLU:HG3	1:B:286:ILE:HD13	1.78	0.66
1:A:160:GLU:HB3	1:B:42:PHE:HZ	1.59	0.66
1:A:107:LEU:HD21	1:A:127:GLN:CB	2.23	0.66
1:A:248:GLU:OE2	1:A:299:PHE:HB3	1.95	0.66
1:A:45:PHE:HB3	1:A:46:PRO:HA	1.78	0.65
1:B:172:ALA:O	1:B:176:ILE:HB	1.97	0.65
1:B:151:LYS:O	1:B:156:PHE:HD2	1.79	0.65
1:A:182:THR:OG1	1:A:185:GLU:HG3	1.96	0.65
1:B:99:SER:O	1:B:102:ILE:HG12	1.97	0.64
1:A:197:PHE:O	1:A:198:PHE:HB2	1.96	0.64
1:B:187:VAL:O	1:B:190:PHE:HB3	1.97	0.64
1:A:184:GLY:O	1:A:188:VAL:HG23	1.98	0.64
1:A:44:ILE:CG2	1:A:45:PHE:H	2.10	0.63
1:B:178:ASP:OD2	1:B:180:LYS:HB2	1.99	0.63
1:A:262:GLU:HG3	1:A:286:ILE:HD13	1.80	0.63
1:A:33:PRO:HD2	4:A:354:HOH:O	1.99	0.62
1:A:44:ILE:HG23	1:A:45:PHE:CD2	2.35	0.62
1:A:45:PHE:CE2	1:B:136:GLU:HG3	2.35	0.61
1:A:107:LEU:CD2	1:A:127:GLN:HB3	2.25	0.61
1:B:127:GLN:HG3	1:B:231:HIS:CE1	2.35	0.61
1:B:162:MET:SD	1:B:163:PRO:HD2	2.40	0.61
1:A:256:VAL:HG12	1:A:303:PHE:CZ	2.36	0.61
1:B:148:ASP:O	1:B:151:LYS:HG2	2.00	0.61
1:B:155:LEU:HD23	1:B:156:PHE:CE2	2.36	0.61
1:B:168:LYS:HE3	1:B:197:PHE:CD2	2.36	0.61
1:B:127:GLN:O	1:B:131:GLU:HG2	2.01	0.60
1:B:138:TYR:O	1:B:142:ILE:HG12	2.00	0.60
1:A:73:LYS:HE2	1:A:77:HIS:NE2	2.16	0.60
1:A:253:GLU:O	1:A:257:ASP:HB2	2.02	0.60
1:B:40:ARG:NH2	1:B:44:ILE:O	2.35	0.60
1:A:252:ARG:HD2	1:A:302:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HG11	1:B:299:PHE:CE2	2.37	0.59
1:B:291:ASP:OD1	1:B:303:PHE:HD2	1.85	0.59
1:B:267:THR:HG21	1:B:283:LYS:HG3	1.84	0.59
1:A:41:ARG:HH12	1:A:47:ILE:HA	1.66	0.59
1:A:239:PHE:O	1:A:242:LEU:HB2	2.02	0.59
1:B:250:ARG:O	1:B:250:ARG:HD3	2.03	0.59
1:A:109:GLU:O	1:A:113:GLN:HB2	2.02	0.59
1:A:107:LEU:HD11	1:A:124:TYR:HD1	1.67	0.59
1:A:269:ALA:C	1:A:271:PRO:HD3	2.28	0.59
1:A:45:PHE:HD2	1:B:139:SER:HB2	1.68	0.59
1:B:148:ASP:CB	1:B:149:PRO:HD3	2.19	0.58
1:A:160:GLU:HB3	1:B:42:PHE:CZ	2.38	0.58
1:A:41:ARG:HH11	1:A:48:GLN:HG3	1.69	0.58
1:A:155:LEU:O	1:A:159:ILE:HG12	2.03	0.57
1:A:251:VAL:HG21	1:A:299:PHE:CE2	2.39	0.57
1:B:39:SER:CB	1:B:116:GLN:HB3	2.34	0.57
1:B:255:ILE:O	1:B:258:ALA:HB3	2.03	0.57
1:B:40:ARG:NH1	1:B:48:GLN:HB2	2.19	0.57
1:B:206:PHE:CD2	1:B:312:MET:HE1	2.40	0.57
1:A:156:PHE:CZ	1:B:43:VAL:CG2	2.87	0.57
1:A:249:GLU:O	1:A:253:GLU:HG3	2.04	0.57
1:B:210:LYS:HE3	1:B:311:PHE:HB3	1.84	0.57
1:A:39:SER:OG	1:A:117:VAL:HG22	2.05	0.57
1:B:37:LYS:C	1:B:39:SER:N	2.61	0.57
1:B:226:ARG:HA	1:B:317:LEU:HD21	1.87	0.56
1:B:255:ILE:HD12	1:B:294:LEU:CD2	2.34	0.56
1:A:106:ASN:C	1:A:106:ASN:HD22	2.13	0.56
1:A:171:TRP:CZ3	1:A:197:PHE:HE2	2.23	0.56
1:A:44:ILE:CG2	1:A:45:PHE:N	2.61	0.56
1:A:156:PHE:CE2	1:B:43:VAL:CG2	2.89	0.56
1:A:41:ARG:HD3	1:A:48:GLN:OE1	2.05	0.56
1:B:52:ILE:HG23	1:B:234:PHE:CE1	2.39	0.56
1:B:207:TRP:CD1	1:B:277:MET:HG3	2.40	0.56
1:A:105:GLU:CB	1:A:108:VAL:CG1	2.82	0.55
1:A:176:ILE:HD11	1:A:189:ALA:HB1	1.87	0.55
1:A:181:SER:HA	1:A:185:GLU:OE1	2.06	0.55
1:B:40:ARG:CZ	1:B:48:GLN:CG	2.84	0.55
1:B:39:SER:OG	1:B:116:GLN:HB2	2.07	0.55
1:A:105:GLU:HB3	1:A:108:VAL:HG11	1.86	0.55
1:A:110:ARG:NH2	1:A:186:ARG:HD3	2.21	0.55
1:A:207:TRP:HD1	1:A:275:ILE:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLU:HG3	1:B:268:GLU:OE2	2.07	0.55
1:A:171:TRP:CE3	1:A:197:PHE:HE2	2.25	0.55
1:A:110:ARG:NH2	1:A:186:ARG:CD	2.68	0.55
1:A:156:PHE:CZ	1:B:43:VAL:HG23	2.42	0.54
1:B:183:PHE:O	1:B:187:VAL:HG23	2.07	0.54
1:A:45:PHE:CZ	1:B:136:GLU:HG3	2.43	0.54
1:A:110:ARG:HH21	1:A:186:ARG:NE	2.06	0.54
1:A:159:ILE:C	1:A:161:THR:H	2.15	0.54
1:A:183:PHE:O	1:A:187:VAL:HG23	2.08	0.54
1:B:153:GLU:C	1:B:153:GLU:CD	2.76	0.54
1:A:263:GLN:O	1:A:267:THR:HG23	2.08	0.54
1:B:257:ASP:O	1:B:261:ILE:HG12	2.08	0.54
1:A:107:LEU:HD22	1:A:127:GLN:CG	2.38	0.54
1:B:102:ILE:C	1:B:104:ASN:H	2.15	0.54
1:A:92:ILE:HG13	1:A:93:LEU:N	2.23	0.53
1:B:291:ASP:HA	1:B:294:LEU:HD12	1.89	0.53
1:B:167:LYS:HB3	1:B:261:ILE:HD12	1.91	0.53
1:A:160:GLU:CD	1:B:42:PHE:HZ	2.17	0.53
1:A:41:ARG:NH1	1:A:48:GLN:HG3	2.22	0.53
1:A:107:LEU:HD22	1:A:127:GLN:HG2	1.91	0.53
1:A:292:ARG:O	1:A:295:VAL:HG12	2.09	0.52
1:B:251:VAL:HG11	1:B:299:PHE:HE2	1.74	0.52
1:B:312:MET:HA	1:B:312:MET:CE	2.37	0.52
1:B:103:VAL:HG12	1:B:103:VAL:O	2.09	0.52
1:B:159:ILE:C	1:B:165:VAL:HG11	2.34	0.52
1:A:71:LEU:CA	1:A:74:ASP:OD2	2.58	0.52
1:B:93:LEU:HB3	1:B:142:ILE:HD11	1.91	0.52
1:A:44:ILE:HG22	1:B:139:SER:CB	2.40	0.52
1:B:292:ARG:O	1:B:295:VAL:HG12	2.09	0.52
1:A:160:GLU:CD	1:B:42:PHE:CZ	2.88	0.52
1:B:163:PRO:HB2	1:B:167:LYS:NZ	2.25	0.52
1:B:164:TYR:O	1:B:168:LYS:HB2	2.09	0.52
1:A:120:ALA:O	1:A:124:TYR:CD2	2.63	0.51
1:A:269:ALA:O	1:A:271:PRO:HD3	2.10	0.51
1:B:104:ASN:HD21	1:B:131:GLU:CG	2.24	0.51
1:A:113:GLN:HG3	1:B:109:GLU:CD	2.36	0.51
1:B:149:PRO:HG3	1:B:152:ARG:NH2	2.26	0.51
1:B:104:ASN:ND2	1:B:131:GLU:HG3	2.26	0.50
1:B:41:ARG:H	1:B:41:ARG:CD	2.10	0.50
1:B:197:PHE:O	1:B:262:GLU:OE1	2.29	0.50
1:A:158:ALA:O	1:A:161:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:O	1:A:250:ARG:HD3	2.12	0.50
1:A:160:GLU:OE2	1:B:42:PHE:CZ	2.63	0.50
1:A:120:ALA:O	1:A:124:TYR:HD2	1.94	0.50
1:A:140:LEU:O	1:A:144:THR:CG2	2.59	0.50
1:A:107:LEU:HD11	1:A:124:TYR:CD1	2.45	0.50
1:A:156:PHE:CE2	1:B:43:VAL:HG23	2.47	0.50
1:A:166:LYS:HA	1:A:166:LYS:CE	2.27	0.49
1:B:74:ASP:O	1:B:77:HIS:HB2	2.12	0.49
1:B:184:GLY:CA	1:B:242:LEU:HD21	2.32	0.49
1:B:314:ASN:ND2	1:B:317:LEU:HB2	2.26	0.49
1:A:70:ASP:OD1	1:A:72:SER:OG	2.24	0.49
1:A:75:LEU:HD11	4:A:360:HOH:O	2.13	0.49
1:A:110:ARG:HH21	1:A:186:ARG:CZ	2.26	0.49
1:A:113:GLN:HG3	1:B:109:GLU:OE2	2.12	0.49
1:A:32:GLU:O	1:A:36:ARG:N	2.45	0.49
1:A:45:PHE:CB	1:A:46:PRO:HA	2.38	0.49
1:B:163:PRO:HB2	1:B:167:LYS:HZ3	1.77	0.49
1:B:271:PRO:C	1:B:273:GLY:H	2.20	0.49
1:A:106:ASN:C	1:A:106:ASN:ND2	2.71	0.49
1:B:77:HIS:CB	1:B:214:MET:HE3	2.42	0.49
1:B:278:ASN:HB3	1:B:281:LEU:HD12	1.95	0.48
1:A:176:ILE:HD11	1:A:189:ALA:CB	2.44	0.48
1:B:251:VAL:HG21	1:B:299:PHE:CE2	2.48	0.48
1:A:162:MET:O	1:A:165:VAL:CG1	2.61	0.48
1:B:200:GLY:HA3	1:B:266:LEU:CD1	2.43	0.48
1:A:44:ILE:CG2	1:A:45:PHE:CD2	2.97	0.48
1:A:156:PHE:CE2	1:B:43:VAL:HG21	2.49	0.48
1:B:92:ILE:HD13	1:B:201:SER:HB3	1.96	0.48
1:B:151:LYS:O	1:B:155:LEU:HB3	2.12	0.48
1:A:107:LEU:CD2	1:A:127:GLN:HG2	2.44	0.47
1:B:45:PHE:HA	1:B:46:PRO:C	2.39	0.47
1:B:206:PHE:CG	1:B:312:MET:HE1	2.48	0.47
1:B:140:LEU:O	1:B:144:THR:HG23	2.14	0.47
1:B:201:SER:O	1:B:205:ILE:HG13	2.15	0.47
1:A:57:LYS:NZ	1:B:136:GLU:OE2	2.48	0.47
1:A:119:GLU:OE2	1:A:119:GLU:N	2.40	0.47
1:A:95:PHE:CE1	1:A:159:ILE:HD12	2.50	0.46
1:B:146:ILE:CG2	1:B:151:LYS:HD3	2.45	0.46
1:A:41:ARG:NH2	1:A:119:GLU:OE1	2.49	0.46
1:B:32:GLU:O	1:B:36:ARG:HG3	2.15	0.46
1:B:93:LEU:HB3	1:B:142:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:MET:SD	1:B:269:ALA:HB1	2.55	0.46
1:A:179:ARG:C	1:A:181:SER:H	2.23	0.46
1:B:117:VAL:O	1:B:121:ARG:HG2	2.15	0.46
1:A:52:ILE:CD1	1:A:238:MET:HE1	2.45	0.46
1:A:107:LEU:CD2	1:A:127:GLN:CG	2.93	0.46
1:B:40:ARG:NH2	1:B:48:GLN:HG2	2.31	0.46
1:B:247:SER:C	1:B:249:GLU:H	2.24	0.46
1:A:44:ILE:CG2	1:B:139:SER:CB	2.93	0.46
1:B:52:ILE:HG12	1:B:238:MET:HE1	1.98	0.46
1:B:200:GLY:HA3	1:B:266:LEU:HD11	1.97	0.46
1:B:204:ALA:O	1:B:207:TRP:HB3	2.16	0.46
1:A:130:ILE:HD13	1:A:130:ILE:HA	1.83	0.46
1:B:271:PRO:C	1:B:273:GLY:N	2.74	0.46
1:A:45:PHE:HE2	1:B:136:GLU:HG3	1.80	0.45
1:A:252:ARG:HD2	1:A:302:VAL:CB	2.45	0.45
1:B:110:ARG:NH2	1:B:186:ARG:CZ	2.79	0.45
1:A:105:GLU:CG	1:A:108:VAL:HG11	2.47	0.45
1:A:160:GLU:CB	1:B:42:PHE:HZ	2.28	0.45
1:A:179:ARG:HA	1:A:179:ARG:HD2	1.80	0.45
1:B:39:SER:CB	1:B:116:GLN:CB	2.94	0.45
1:B:149:PRO:C	1:B:151:LYS:N	2.74	0.45
1:A:127:GLN:HG3	1:A:231:HIS:CE1	2.51	0.45
1:A:162:MET:HB3	1:A:163:PRO:CD	2.46	0.45
1:A:259:VAL:HG13	1:A:286:ILE:HG22	1.98	0.45
1:B:102:ILE:C	1:B:104:ASN:N	2.75	0.45
1:B:287:GLU:CD	1:B:303:PHE:CD1	2.95	0.45
1:A:147:ARG:HD3	1:A:147:ARG:N	2.05	0.45
1:B:149:PRO:HG3	1:B:152:ARG:HH22	1.81	0.45
1:B:247:SER:C	1:B:249:GLU:N	2.74	0.45
1:A:45:PHE:HD2	1:B:139:SER:CB	2.29	0.45
1:A:251:VAL:HG21	1:A:299:PHE:CZ	2.52	0.44
1:B:295:VAL:HG13	1:B:296:GLU:N	2.32	0.44
1:B:312:MET:C	1:B:313:GLU:OE1	2.61	0.44
1:B:296:GLU:OE1	1:B:296:GLU:HA	2.18	0.44
1:A:105:GLU:HB3	1:A:108:VAL:HG12	1.96	0.44
1:B:78:TRP:CE2	1:B:86:LYS:HD2	2.53	0.44
1:B:303:PHE:O	1:B:304:GLN:HB2	2.18	0.44
1:B:96:PHE:CZ	1:B:201:SER:HB2	2.53	0.44
1:A:43:VAL:CG1	1:A:44:ILE:N	2.72	0.43
1:A:159:ILE:C	1:A:161:THR:N	2.76	0.43
1:B:255:ILE:HD12	1:B:294:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TYR:HB2	1:B:309:PHE:CE2	2.53	0.43
1:B:296:GLU:C	1:B:298:GLY:H	2.26	0.43
1:A:32:GLU:HG3	4:A:354:HOH:O	2.19	0.43
1:B:49:TYR:CD2	1:B:49:TYR:N	2.86	0.43
1:A:73:LYS:O	1:A:73:LYS:HG2	2.19	0.43
1:B:110:ARG:NH2	1:B:186:ARG:NH1	2.66	0.43
1:B:118:PRO:HG2	1:B:119:GLU:OE2	2.19	0.43
1:B:146:ILE:HG22	1:B:151:LYS:HD3	2.01	0.43
1:A:36:ARG:HG2	1:A:38:SER:OG	2.19	0.43
1:B:302:VAL:O	1:B:302:VAL:HG22	2.17	0.43
1:A:162:MET:HB3	1:A:163:PRO:HD2	1.99	0.43
1:B:255:ILE:HD12	1:B:294:LEU:HD21	1.99	0.43
1:A:220:SER:O	1:A:224:ILE:HG13	2.18	0.43
1:A:109:GLU:O	1:A:113:GLN:CG	2.67	0.42
1:B:124:TYR:CZ	1:B:234:PHE:HE2	2.36	0.42
1:B:113:GLN:HE21	1:B:113:GLN:HB3	1.58	0.42
1:B:58:GLN:HE21	1:B:58:GLN:HB2	1.63	0.42
1:A:52:ILE:HD13	1:A:238:MET:HE1	2.00	0.42
1:A:289:VAL:HG22	1:A:292:ARG:NH2	2.34	0.42
1:B:137:MET:HA	1:B:137:MET:CE	2.45	0.42
1:B:196:VAL:HG22	1:B:289:VAL:HG12	2.01	0.42
1:B:303:PHE:O	1:B:304:GLN:CB	2.66	0.42
1:A:105:GLU:CB	1:A:108:VAL:HG11	2.47	0.42
1:B:250:ARG:HD3	1:B:250:ARG:C	2.45	0.42
1:A:302:VAL:HG22	1:A:302:VAL:O	2.20	0.41
1:B:131:GLU:OE2	1:B:131:GLU:HA	2.20	0.41
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.69	0.41
1:B:110:ARG:HH22	1:B:186:ARG:NH2	2.17	0.41
1:B:210:LYS:CE	1:B:311:PHE:HB3	2.49	0.41
1:A:262:GLU:CG	1:A:286:ILE:HD13	2.49	0.41
1:A:41:ARG:NH2	1:A:119:GLU:CD	2.78	0.41
1:A:183:PHE:HA	1:A:186:ARG:NH2	2.36	0.41
1:B:118:PRO:HA	1:B:121:ARG:HG3	2.02	0.41
1:A:253:GLU:O	1:A:257:ASP:CB	2.68	0.41
1:B:41:ARG:N	1:B:41:ARG:CD	2.76	0.41
1:B:190:PHE:CD2	1:B:235:ALA:HB2	2.56	0.41
1:B:288:PHE:CE2	1:B:307:ASN:HB2	2.56	0.41
1:A:92:ILE:CD1	1:A:205:ILE:HD11	2.50	0.41
1:B:252:ARG:HH11	1:B:302:VAL:HB	1.86	0.41
1:A:152:ARG:O	1:A:155:LEU:HB3	2.21	0.40
1:B:31:GLU:H	1:B:31:GLU:HG2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:SER:O	1:B:40:ARG:O	2.38	0.40
1:A:108:VAL:HG13	1:A:109:GLU:N	2.37	0.40
1:A:255:ILE:HD12	1:A:293:LEU:HD23	2.03	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	275/351 (78%)	248 (90%)	26 (10%)	1 (0%)	30	51
1	B	282/351 (80%)	254 (90%)	27 (10%)	1 (0%)	30	51
All	All	557/702 (79%)	502 (90%)	53 (10%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	ASP
1	A	44	ILE

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	247/310 (80%)	234 (95%)	13 (5%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	252/310 (81%)	231 (92%)	21 (8%)	10	23
All	All	499/620 (80%)	465 (93%)	34 (7%)	14	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	MET
1	A	85	GLU
1	A	144	THR
1	A	147	ARG
1	A	166	LYS
1	A	173	LEU
1	A	214	MET
1	A	223	LEU
1	A	242	LEU
1	A	245	LYS
1	A	247	SER
1	A	270	LEU
1	A	310	ASP
1	B	34	LEU
1	B	40	ARG
1	B	49	TYR
1	B	51	ASP
1	B	55	MET
1	B	67	GLU
1	B	92	ILE
1	B	113	GLN
1	B	121	ARG
1	B	137	MET
1	B	140	LEU
1	B	147	ARG
1	B	197	PHE
1	B	214	MET
1	B	223	LEU
1	B	230	LEU
1	B	242	LEU
1	B	245	LYS
1	B	312	MET
1	B	313	GLU
1	B	314	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	79	ASN
1	A	106	ASN
1	A	116	GLN
1	A	127	GLN
1	A	132	ASN
1	A	240	GLN
1	A	284	GLN
1	A	304	GLN
1	B	58	GLN
1	B	60	GLN
1	B	104	ASN
1	B	113	GLN
1	B	127	GLN
1	B	132	ASN
1	B	263	GLN
1	B	314	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	SO4	A	502	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	B	501	-	4,4,4	0.38	0	6,6,6	0.11	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, 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	279/351 (79%)	0.80	33 (11%) 9 7	22, 58, 97, 121	0
1	B	286/351 (81%)	1.19	65 (22%) 2 1	28, 65, 117, 137	0
All	All	565/702 (80%)	1.00	98 (17%) 4 3	22, 62, 112, 137	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	PHE	7.9
1	A	43	VAL	7.8
1	A	42	PHE	7.2
1	A	109	GLU	7.0
1	B	42	PHE	6.9
1	B	315	ILE	6.9
1	A	108	VAL	6.2
1	B	173	LEU	6.1
1	B	102	ILE	5.9
1	B	103	VAL	5.8
1	B	152	ARG	5.6
1	B	159	ILE	5.4
1	B	317	LEU	5.3
1	A	107	LEU	5.2
1	B	43	VAL	5.2
1	B	175	TRP	4.6
1	B	41	ARG	4.5
1	B	172	ALA	4.5
1	A	40	ARG	4.4
1	B	39	SER	4.3
1	B	158	ALA	4.2
1	A	44	ILE	4.2
1	A	124	TYR	4.1
1	A	41	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	157	ASN	4.0
1	B	153	GLU	4.0
1	B	156	PHE	3.9
1	B	38	SER	3.9
1	A	73	LYS	3.9
1	B	111	PHE	3.8
1	B	109	GLU	3.8
1	B	177	ALA	3.7
1	A	311	PHE	3.6
1	A	39	SER	3.6
1	A	105	GLU	3.5
1	B	98	ALA	3.5
1	A	179	ARG	3.5
1	B	174	ARG	3.5
1	B	30	ASN	3.5
1	B	198	PHE	3.4
1	A	80	LYS	3.4
1	B	154	PHE	3.4
1	A	29	SER	3.4
1	B	162	MET	3.3
1	B	190	PHE	3.3
1	B	100	ASP	3.3
1	B	316	SER	3.2
1	B	252	ARG	3.2
1	B	180	LYS	3.2
1	A	158	ALA	3.1
1	B	106	ASN	3.1
1	B	40	ARG	3.1
1	B	303	PHE	3.1
1	B	149	PRO	3.0
1	B	168	LYS	3.0
1	B	155	LEU	3.0
1	B	150	LYS	2.9
1	A	100	ASP	2.8
1	B	164	TYR	2.8
1	B	108	VAL	2.8
1	B	196	VAL	2.8
1	B	37	LYS	2.7
1	A	175	TRP	2.7
1	B	195	GLY	2.7
1	A	74	ASP	2.7
1	B	151	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	181	SER	2.7
1	B	104	ASN	2.7
1	B	171	TRP	2.7
1	A	300	SER	2.6
1	B	146	ILE	2.6
1	A	72	SER	2.6
1	B	99	SER	2.5
1	B	166	LYS	2.5
1	B	260	LYS	2.5
1	B	268	GLU	2.5
1	B	101	GLY	2.5
1	B	147	ARG	2.4
1	B	112	SER	2.4
1	B	169	ALA	2.4
1	B	314	ASN	2.4
1	B	163	PRO	2.3
1	B	251	VAL	2.3
1	A	99	SER	2.3
1	B	302	VAL	2.3
1	A	307	ASN	2.3
1	B	107	LEU	2.2
1	A	180	LYS	2.2
1	A	174	ARG	2.2
1	A	171	TRP	2.2
1	B	246	PRO	2.2
1	B	51	ASP	2.1
1	B	197	PHE	2.1
1	A	310	ASP	2.0
1	A	46	PRO	2.0
1	A	251	VAL	2.0
1	A	177	ALA	2.0
1	B	243	VAL	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, 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
3	SO4	B	501	5/5	0.73	0.12	120,120,120,121	0
2	FE	B	402	1/1	0.78	0.29	142,142,142,142	0
3	SO4	A	502	5/5	0.87	0.16	151,151,151,152	0
2	FE	B	401	1/1	0.97	0.06	79,79,79,79	0
2	FE	A	401	1/1	0.99	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.