



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:28 pm GMT

PDB ID : 3HF1  
Title : Crystal structure of human p53R2  
Authors : Smith, P.; Zhou, B.; Yuan, Y.-C.; Su, L.; Tsai, S.-C.; Yen, Y.  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

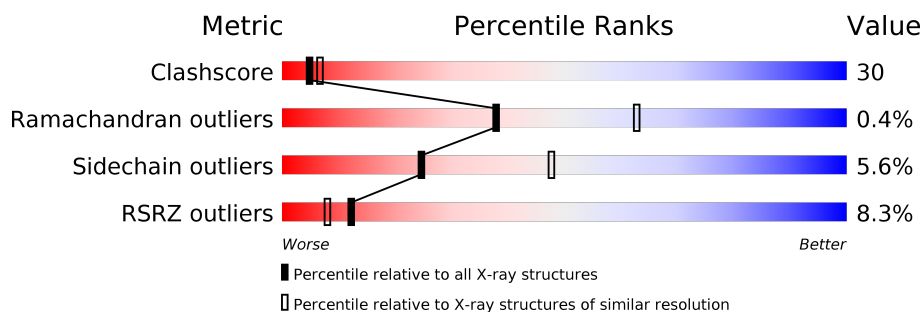
# 1 Overall quality at a glance

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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	502	-	-	-	X

## 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 (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.67Å 99.55Å 132.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 47.62 – 2.61	Depositor EDS
% Data completeness (in resolution range)	88.0 (50.00-2.60) 88.7 (47.62-2.61)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.273 0.240 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.42	0/2366	0.61	0/3193
1	B	0.39	0/2414	0.60	0/3257
All	All	0.41	0/4780	0.61	0/6450

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.

There are no bond angle outliers.

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 [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	2306	0	2282	144	0
1	B	2354	0	2338	162	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	282	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 30.

All (282) 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:H	1:A:147:ARG:HD3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:OD1	1:A:280:ILE:HG22	1.86	0.75
1:B:146:ILE:HG21	1:B:151:LYS:CB	2.17	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
1:B:52:ILE:HG23	1:B:234:PHE:HE1	1.57	0.69
1:B:153:GLU:OE1	1:B:153:GLU:C	2.30	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: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:312:MET:HA	1:B:312:MET:HE2	1.75	0.67
1:B:39:SER:HB2	1:B:116:GLN:HB3	1.76	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:B:206:PHE:CB	1:B:312:MET:HE3	2.30	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:239:PHE:O	1:A:242:LEU:HB2	2.02	0.59
1:A:41:ARG:HH12	1:A:47:ILE:HA	1.66	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: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: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:156:PHE:CZ	1:B:43:VAL:CG2	2.87	0.57
1:A:39:SER:OG	1:A:117:VAL:HG22	2.05	0.57
1:B:255:ILE:HD12	1:B:294:LEU:CD2	2.34	0.56
1:B:226:ARG:HA	1:B:317:LEU:HD21	1.87	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:207:TRP:CD1	1:B:277:MET:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:HG23	1:B:234:PHE:CE1	2.39	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
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:B:238:MET:HA	1:B:238:MET:HE2	1.88	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:269:ALA:C	1:A:271:PRO:HD3	2.28	0.54
1:A:183:PHE:O	1:A:187:VAL:HG23	2.08	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: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:B:77:HIS:HB3	1:B:214:MET:HE3	1.90	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:B:37:LYS:C	1:B:39:SER:N	2.61	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: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:106:ASN:HD22	1:A:106:ASN:C	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:197:PHE:O	1:B:262:GLU:OE1	2.29	0.50
1:B:41:ARG:CD	1:B:41:ARG:H	2.10	0.50
1:A:158:ALA:O	1:A:161:THR:HB	2.12	0.50
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:CE	1:A:166:LYS:HA	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:110:ARG:HH21	1:A:186:ARG:CZ	2.26	0.49
1:A:75:LEU:HD11	4:A:360:HOH:O	2.13	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:102:ILE:C	1:B:104:ASN:H	2.15	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:160:GLU:CD	1:B:42:PHE:HZ	2.17	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:A:159:ILE:C	1:A:161:THR:H	2.15	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:A:160:GLU:CD	1:B:42:PHE:CZ	2.88	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: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:137:MET:HA	1:B:137:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:CG2	1:B:151:LYS:HD3	2.45	0.46
1:B:159:ILE:C	1:B:165:VAL:HG11	2.34	0.46
1:A:41:ARG:NH2	1:A:119:GLU:OE1	2.49	0.46
1:B:93:LEU:HB3	1:B:142:ILE:CD1	2.45	0.46
1:B:162:MET:SD	1:B:269:ALA:HB1	2.55	0.46
1:B:32:GLU:O	1:B:36:ARG:HG3	2.15	0.46
1:B:117:VAL:O	1:B:121:ARG:HG2	2.15	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:A:44:ILE:CG2	1:B:139:SER:CB	2.93	0.46
1:A:113:GLN:HG3	1:B:109:GLU:CD	2.36	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:A:252:ARG:HD2	1:A:302:VAL:CB	2.45	0.45
1:A:45:PHE:HE2	1:B:136:GLU:HG3	1.80	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: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:A:160:GLU:CB	1:B:42:PHE:HZ	2.28	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:A:147:ARG:N	1:A:147:ARG:HD3	2.05	0.45
1:B:149:PRO:HG3	1:B:152:ARG:HH22	1.81	0.45
1:A:45:PHE:HD2	1:B:139:SER:CB	2.29	0.45
1:A:57:LYS:NZ	1:B:136:GLU:OE2	2.48	0.45
1:A:251:VAL:HG21	1:A:299:PHE:CZ	2.52	0.44
1:B:271:PRO:C	1:B:273:GLY:H	2.20	0.44
1:B:295:VAL:HG13	1:B:296:GLU:N	2.32	0.44
1:B:153:GLU:CD	1:B:153:GLU:C	2.76	0.44
1:B:206:PHE:CG	1:B:312:MET:HE3	2.52	0.44
1:B:238:MET:HA	1:B:238:MET:CE	2.48	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:A:106:ASN:ND2	1:A:106:ASN:C	2.71	0.44
1:B:303:PHE:O	1:B:304:GLN:HB2	2.18	0.44
1:B:78:TRP:CE2	1:B:86:LYS:HD2	2.53	0.44
1:B:206:PHE:HB2	1:B:312:MET:HE3	2.00	0.44
1:B:96:PHE:CZ	1:B:201:SER:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:CG1	1:A:44:ILE:N	2.72	0.43
1:B:255:ILE:HD12	1:B:294:LEU:HD23	1.99	0.43
1:B:285:TYR:HB2	1:B:309:PHE:CE2	2.53	0.43
1:A:32:GLU:HG3	4:A:354:HOH:O	2.19	0.43
1:B:238:MET:HE2	1:B:238:MET:CA	2.48	0.43
1:B:49:TYR:CD2	1:B:49:TYR:N	2.86	0.43
1:A:73:LYS:HG2	1:A:73:LYS:O	2.19	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:B:110:ARG:NH2	1:B:186:ARG:NH1	2.66	0.43
1:B:45:PHE:HA	1:B:46:PRO:C	2.39	0.43
1:A:36:ARG:HG2	1:A:38:SER:OG	2.19	0.43
1:B:302:VAL:HG22	1:B:302:VAL:O	2.17	0.43
1:B:137:MET:HA	1:B:137:MET:HE3	1.99	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:303:PHE:O	1:B:304:GLN:CB	2.66	0.42
1:B:113:GLN:HE21	1:B:113:GLN:HB3	1.58	0.42
1:B:58:GLN:HB2	1:B:58:GLN:HE21	1.63	0.42
1:A:289:VAL:HG22	1:A:292:ARG:NH2	2.34	0.42
1:B:196:VAL:HG22	1:B:289:VAL:HG12	2.01	0.42
1:A:105:GLU:CB	1:A:108:VAL:HG11	2.47	0.42
1:A:302:VAL:O	1:A:302:VAL:HG22	2.20	0.41
1:B:131:GLU:HA	1:B:131:GLU:OE2	2.20	0.41
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.69	0.41
1:A:179:ARG:C	1:A:181:SER:H	2.23	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:B:247:SER:C	1:B:249:GLU:H	2.24	0.41
1:A:262:GLU:CG	1:A:286:ILE:HD13	2.49	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:B:271:PRO:C	1:B:273:GLY:N	2.74	0.41
1:A:253:GLU:O	1:A:257:ASP:CB	2.68	0.41
1:B:288:PHE:CE2	1:B:307:ASN:HB2	2.56	0.41
1:B:190:PHE:CD2	1:B:235:ALA:HB2	2.56	0.41
1:B:41:ARG:CD	1:B:41:ARG:N	2.76	0.41
1:A:92:ILE:CD1	1:A:205:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PRO:C	1:B:151:LYS:N	2.74	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
1:B:39:SER:O	1:B:40:ARG:O	2.38	0.40
1:B:102:ILE:C	1:B:104:ASN:N	2.75	0.40
1:B:247:SER:C	1:B:249:GLU:N	2.74	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
1:B:287:GLU:CD	1:B:303:PHE:CD1	2.95	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%)	38	63
1	B	282/351 (80%)	254 (90%)	27 (10%)	1 (0%)	38	63
All	All	557/702 (79%)	502 (90%)	53 (10%)	2 (0%)	38	63

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%)	235 (95%)	12 (5%)	29	54
1	B	252/310 (81%)	236 (94%)	16 (6%)	21	42
All	All	499/620 (80%)	471 (94%)	28 (6%)	25	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	106	ASN
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	270	LEU
1	A	310	ASP
1	B	40	ARG
1	B	41	ARG
1	B	49	TYR
1	B	51	ASP
1	B	92	ILE
1	B	113	GLN
1	B	121	ARG
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	245	LYS
1	B	313	GLU
1	B	314	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	60	GLN
1	A	79	ASN
1	A	106	ASN
1	A	127	GLN
1	A	132	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.33	0	6,6,6	0.07	0
3	SO4	B	501	-	4,4,4	0.34	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	SO4	B	501	-	-	0/0/0/0	0/0/0/0

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	279/351 (79%)	0.23	13 (4%) 32 25	22, 58, 97, 121	0
1	B	286/351 (81%)	0.59	34 (11%) 5 3	28, 65, 117, 137	0
All	All	565/702 (80%)	0.41	47 (8%) 12 8	22, 62, 112, 137	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	GLU	7.0
1	B	174	ARG	6.5
1	B	172	ALA	5.3
1	A	45	PHE	4.5
1	B	153	GLU	4.3
1	B	180	LYS	4.1
1	B	42	PHE	4.1
1	B	152	ARG	4.1
1	B	175	TRP	3.9
1	B	109	GLU	3.8
1	A	107	LEU	3.4
1	B	249	GLU	3.4
1	A	80	LYS	3.3
1	B	176	ILE	3.3
1	B	181	SER	3.3
1	B	173	LEU	3.3
1	A	43	VAL	3.2
1	A	303	PHE	3.1
1	B	179	ARG	3.1
1	B	157	ASN	2.9
1	A	44	ILE	2.8
1	B	171	TRP	2.8
1	B	41	ARG	2.8
1	B	246	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	245	LYS	2.7
1	B	154	PHE	2.7
1	B	252	ARG	2.7
1	A	304	GLN	2.6
1	B	250	ARG	2.6
1	B	111	PHE	2.6
1	A	302	VAL	2.5
1	B	251	VAL	2.5
1	A	108	VAL	2.5
1	B	31	GLU	2.5
1	B	39	SER	2.5
1	B	185	GLU	2.5
1	B	163	PRO	2.4
1	B	297	LEU	2.4
1	B	80	LYS	2.3
1	A	179	ARG	2.3
1	A	39	SER	2.2
1	A	249	GLU	2.2
1	B	43	VAL	2.2
1	B	177	ALA	2.1
1	B	156	PHE	2.1
1	B	82	LYS	2.0
1	B	299	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	502	5/5	0.77	0.23	2.40	151,151,151,152	0
2	FE	A	401	1/1	0.98	0.11	-2.54	62,62,62,62	0
2	FE	B	401	1/1	0.97	0.10	-2.96	79,79,79,79	0
3	SO4	B	501	5/5	0.83	0.27	-	120,120,120,121	0
2	FE	B	402	1/1	0.58	0.41	-	142,142,142,142	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.