



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:49 am BST

PDB ID : 1KT1  
Title : Structure of the Large FKBP-like Protein, FKBP51, Involved in Steroid Receptor Complexes  
Authors : Sinars, C.R.; Cheung-Flynn, J.; Rimerman, R.A.; Scammell, J.G.; Smith, D.F.; Clardy, J.C.  
Deposited on : 2002-01-14  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

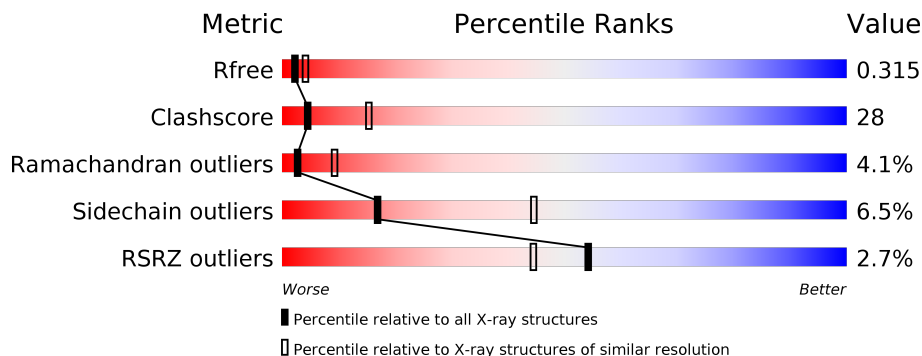
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	457	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3012 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 FK506-binding protein FKBP51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2971	1885	515	553	18	71	1	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

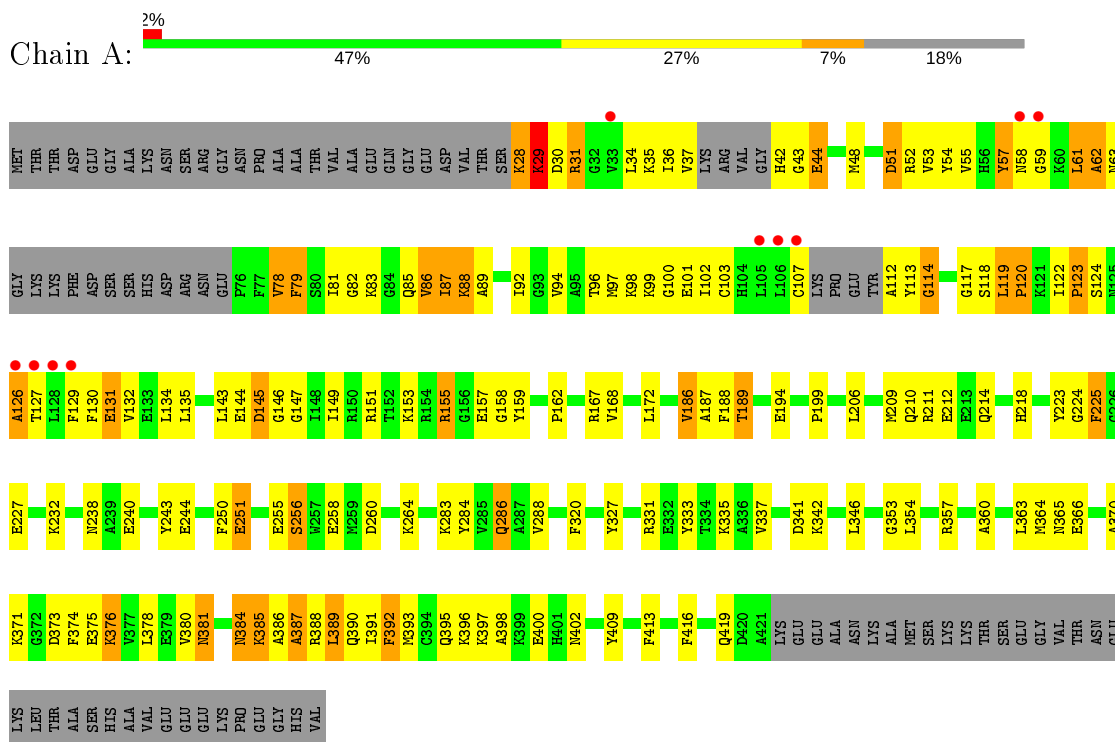
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: FK506-binding protein FKBP51



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.03Å 91.03Å 132.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.05 – 2.80 43.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.05-2.80) 100.0 (43.05-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.314 0.254 , 0.315	Depositor DCC
$R_{free}$ test set	812 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: 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	0.75	7/3023 (0.2%)	0.80	6/4042 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CB-CG	-19.18	1.15	1.52
1	A	395	GLN	CG-CD	-15.89	1.14	1.51
1	A	88	LYS	CB-CG	9.57	1.78	1.52
1	A	29	LYS	CB-CG	8.94	1.76	1.52
1	A	251	GLU	CB-CG	-6.64	1.39	1.52
1	A	44	GLU	CB-CG	6.26	1.64	1.52
1	A	35	LYS	CB-CG	5.02	1.66	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LYS	CA-CB-CG	14.75	145.85	113.40
1	A	28	LYS	CB-CG-CD	6.71	129.05	111.60
1	A	62	ALA	N-CA-C	-6.43	93.63	111.00
1	A	251	GLU	CA-CB-CG	6.12	126.86	113.40
1	A	131	GLU	CA-CB-CG	5.82	126.19	113.40
1	A	225	PHE	N-CA-C	-5.30	96.69	111.00

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	2971	0	2964	164	1
2	A	10	0	0	1	0
3	A	31	0	0	2	0
All	All	3012	0	2964	164	1

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 28.

All (164) 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:A:87:ILE:HD12	1:A:87:ILE:H	1.27	0.96
1:A:87:ILE:HG22	1:A:89:ALA:H	1.38	0.88
1:A:55:VAL:HG12	1:A:134:LEU:HA	1.55	0.87
1:A:206:LEU:HA	1:A:209:MET:HE3	1.56	0.86
1:A:354:LEU:HD13	1:A:376:LYS:HB3	1.58	0.84
1:A:118:SER:HB2	1:A:122:ILE:HB	1.60	0.84
1:A:255:GLU:HG2	1:A:258:GLU:OE2	1.81	0.80
1:A:157:GLU:HG3	1:A:212:GLU:OE1	1.82	0.80
1:A:94:VAL:HG13	1:A:97:MET:HE3	1.67	0.77
1:A:31:ARG:HD2	1:A:34:LEU:HD11	1.68	0.75
1:A:333:TYR:CE2	1:A:363:LEU:HD13	2.21	0.75
1:A:94:VAL:HA	1:A:97:MET:HE3	1.71	0.73
1:A:416:PHE:O	1:A:419:GLN:HB2	1.89	0.72
1:A:59:GLY:HA2	1:A:129:PHE:O	1.90	0.71
1:A:87:ILE:H	1:A:87:ILE:CD1	2.02	0.70
1:A:94:VAL:HA	1:A:97:MET:CE	2.22	0.70
1:A:113:TYR:CD2	1:A:114:GLY:N	2.60	0.70
1:A:153:LYS:HB3	1:A:214:GLN:HG2	1.73	0.69
1:A:283:LYS:HB3	1:A:286:GLN:CG	2.23	0.69
1:A:331:ARG:HH11	1:A:331:ARG:HG2	1.60	0.67
1:A:102:ILE:H	1:A:102:ILE:HD12	1.60	0.67
1:A:61:LEU:HD13	1:A:126:ALA:HB1	1.77	0.67
1:A:54:TYR:HE2	1:A:78:VAL:HG21	1.60	0.67
1:A:167:ARG:HH11	1:A:189:THR:HG22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:C	1:A:384:ASN:HD22	1.98	0.65
1:A:283:LYS:HB3	1:A:286:GLN:HG2	1.78	0.65
1:A:168:VAL:HG12	1:A:250:PHE:HB3	1.79	0.65
1:A:409:TYR:O	1:A:413:PHE:HB2	1.97	0.65
1:A:416:PHE:HA	1:A:419:GLN:HG3	1.78	0.65
1:A:389:LEU:HD12	1:A:389:LEU:O	1.97	0.64
1:A:283:LYS:O	1:A:286:GLN:HG2	1.99	0.62
1:A:341:ASP:OD2	1:A:357:ARG:NH1	2.31	0.62
1:A:168:VAL:HG12	1:A:250:PHE:CB	2.30	0.62
1:A:81:ILE:HG22	1:A:82:GLY:H	1.65	0.61
1:A:87:ILE:N	1:A:87:ILE:HD12	2.09	0.61
1:A:211:ARG:HG2	1:A:212:GLU:HG3	1.82	0.61
1:A:61:LEU:HG	1:A:62:ALA:N	2.16	0.61
1:A:52:ARG:HG2	1:A:52:ARG:HH11	1.65	0.60
1:A:381:ASN:C	1:A:381:ASN:HD22	2.04	0.60
1:A:100:GLY:O	1:A:102:ILE:HD12	2.02	0.60
1:A:119:LEU:CD2	1:A:119:LEU:H	2.15	0.60
1:A:118:SER:HB2	1:A:122:ILE:CB	2.32	0.59
1:A:388:ARG:HA	1:A:391:ILE:HD12	1.84	0.59
1:A:31:ARG:HD2	1:A:34:LEU:CD1	2.32	0.59
1:A:36:ILE:O	1:A:103:CYS:HB2	2.03	0.59
1:A:384:ASN:CG	1:A:387:ALA:HB2	2.23	0.58
1:A:54:TYR:HD2	1:A:78:VAL:HB	1.68	0.58
1:A:58:ASN:O	1:A:130:PHE:HA	2.04	0.58
1:A:31:ARG:CD	1:A:34:LEU:HD11	2.33	0.58
1:A:331:ARG:NH1	1:A:331:ARG:HG2	2.19	0.58
1:A:232:LYS:HB3	1:A:232:LYS:HZ3	1.69	0.57
1:A:61:LEU:HG	1:A:62:ALA:H	1.70	0.57
1:A:86:VAL:HG22	1:A:87:ILE:HD12	1.87	0.57
1:A:353:GLY:O	1:A:357:ARG:HB2	2.05	0.56
1:A:155:ARG:NH1	3:A:506:HOH:O	2.38	0.56
1:A:43:GLY:O	1:A:98:LYS:HD3	2.05	0.56
1:A:389:LEU:O	1:A:392:PHE:HB3	2.06	0.56
1:A:94:VAL:HG13	1:A:97:MET:CE	2.34	0.56
1:A:371:LYS:HB2	1:A:371:LYS:NZ	2.20	0.55
1:A:83:LYS:C	1:A:85:GLN:H	2.10	0.55
1:A:119:LEU:CD2	1:A:119:LEU:N	2.70	0.55
1:A:333:TYR:CZ	1:A:363:LEU:HD13	2.41	0.55
1:A:384:ASN:HD22	1:A:385:LYS:N	2.05	0.55
1:A:79:PHE:CD2	1:A:79:PHE:N	2.74	0.55
1:A:146:GLY:HA2	1:A:149:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:HD2	1:A:79:PHE:H	1.56	0.54
1:A:396:LYS:O	1:A:400:GLU:HG3	2.07	0.54
1:A:42:HIS:ND1	1:A:43:GLY:N	2.54	0.54
1:A:375:GLU:HA	1:A:375:GLU:OE1	2.08	0.53
1:A:386:ALA:O	1:A:390:GLN:HG2	2.08	0.53
1:A:54:TYR:CE2	1:A:78:VAL:HG21	2.40	0.53
1:A:48:MET:HE3	1:A:151:ARG:CZ	2.39	0.52
1:A:162:PRO:HG3	1:A:250:PHE:CD2	2.43	0.52
1:A:53:VAL:HG21	1:A:81:ILE:HD11	1.91	0.52
1:A:393:MET:HE2	1:A:397:LYS:HE2	1.92	0.52
1:A:232:LYS:HB3	1:A:232:LYS:NZ	2.25	0.52
1:A:378:LEU:HD13	1:A:388:ARG:NH1	2.25	0.52
1:A:119:LEU:HD23	1:A:119:LEU:N	2.26	0.50
1:A:337:VAL:HG21	1:A:364:MET:HE3	1.93	0.50
1:A:172:LEU:HD11	1:A:243:TYR:CD2	2.46	0.50
1:A:54:TYR:CD2	1:A:78:VAL:HB	2.45	0.50
1:A:143:LEU:O	1:A:144:GLU:C	2.48	0.50
1:A:119:LEU:N	1:A:122:ILE:O	2.44	0.50
1:A:81:ILE:HG22	1:A:82:GLY:N	2.25	0.49
1:A:28:LYS:O	1:A:30:ASP:N	2.45	0.49
1:A:44:GLU:HA	1:A:98:LYS:CE	2.43	0.49
1:A:381:ASN:C	1:A:381:ASN:ND2	2.66	0.49
1:A:86:VAL:HG22	1:A:87:ILE:CD1	2.42	0.48
1:A:127:THR:O	1:A:127:THR:HG22	2.13	0.48
1:A:158:GLY:O	1:A:210:GLN:NE2	2.46	0.48
1:A:79:PHE:HD2	1:A:79:PHE:N	2.10	0.48
1:A:337:VAL:HG21	1:A:364:MET:CE	2.43	0.48
1:A:82:GLY:O	1:A:155:ARG:NH2	2.47	0.48
1:A:54:TYR:O	1:A:135:LEU:HB2	2.14	0.47
1:A:378:LEU:HD21	1:A:387:ALA:HB3	1.96	0.47
1:A:211:ARG:O	1:A:212:GLU:HB2	2.15	0.47
1:A:153:LYS:CD	1:A:214:GLN:HE21	2.28	0.47
1:A:57:TYR:HD2	1:A:57:TYR:H	1.62	0.47
1:A:44:GLU:HA	1:A:98:LYS:HE2	1.97	0.47
1:A:153:LYS:HD3	1:A:214:GLN:HE21	1.79	0.46
1:A:370:ALA:O	1:A:373:ASP:HB2	2.15	0.46
1:A:232:LYS:HD2	2:A:601:SO4:O3	2.15	0.46
1:A:42:HIS:CB	1:A:99:LYS:O	2.63	0.46
1:A:378:LEU:HD11	1:A:388:ARG:HG2	1.97	0.46
1:A:87:ILE:HG22	1:A:88:LYS:N	2.31	0.46
1:A:92:ILE:O	1:A:96:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:OE2	1:A:238:ASN:ND2	2.46	0.46
1:A:62:ALA:O	1:A:63:ASN:HB3	2.16	0.45
1:A:218[B]:HIS:NE2	1:A:240:GLU:OE1	2.49	0.45
1:A:57:TYR:HA	1:A:131:GLU:O	2.17	0.45
1:A:42:HIS:CG	1:A:43:GLY:H	2.35	0.45
1:A:119:LEU:HA	1:A:122:ILE:H	1.82	0.45
1:A:87:ILE:HG22	1:A:89:ALA:N	2.20	0.45
1:A:145:ASP:OD1	1:A:147:GLY:N	2.49	0.45
1:A:57:TYR:CD2	1:A:57:TYR:N	2.85	0.45
1:A:162:PRO:HG3	1:A:250:PHE:CG	2.52	0.44
1:A:364:MET:O	1:A:365:ASN:HB2	2.17	0.44
1:A:188:PHE:HB2	3:A:522:HOH:O	2.17	0.44
1:A:94:VAL:HA	1:A:97:MET:HE2	1.98	0.44
1:A:119:LEU:HD22	1:A:119:LEU:H	1.82	0.44
1:A:376:LYS:HB2	1:A:376:LYS:HE2	1.90	0.44
1:A:61:LEU:CG	1:A:62:ALA:N	2.80	0.43
1:A:337:VAL:CG2	1:A:364:MET:HE1	2.49	0.43
1:A:61:LEU:C	1:A:63:ASN:H	2.03	0.43
1:A:94:VAL:CG1	1:A:97:MET:HE3	2.42	0.43
1:A:118:SER:HB2	1:A:122:ILE:CG2	2.49	0.43
1:A:398:ALA:O	1:A:402:ASN:ND2	2.49	0.43
1:A:42:HIS:HB3	1:A:99:LYS:O	2.18	0.43
1:A:53:VAL:O	1:A:78:VAL:HA	2.18	0.43
1:A:199:PRO:HG3	1:A:225:PHE:CZ	2.53	0.43
1:A:320:PHE:CE1	1:A:342:LYS:HB3	2.54	0.43
1:A:53:VAL:CG1	1:A:54:TYR:N	2.81	0.43
1:A:53:VAL:O	1:A:78:VAL:HG23	2.19	0.43
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.82	0.43
1:A:53:VAL:CG1	1:A:55:VAL:HG13	2.49	0.42
1:A:88:LYS:O	1:A:92:ILE:HG13	2.19	0.42
1:A:153:LYS:HE3	1:A:244:GLU:OE2	2.19	0.42
1:A:145:ASP:OD1	1:A:145:ASP:C	2.57	0.42
1:A:371:LYS:HE3	1:A:391:ILE:CG2	2.49	0.42
1:A:119:LEU:HB2	1:A:120:PRO:HA	2.00	0.42
1:A:168:VAL:HG12	1:A:250:PHE:HB2	2.00	0.42
1:A:224:GLY:C	1:A:225:PHE:O	2.55	0.42
1:A:256:SER:O	1:A:264:LYS:HE2	2.19	0.42
1:A:194:GLU:CG	1:A:283:LYS:NZ	2.82	0.42
1:A:374:PHE:HB2	1:A:391:ILE:HG12	2.01	0.42
1:A:97:MET:HA	1:A:101:GLU:CD	2.39	0.42
1:A:327:TYR:CD1	1:A:335:LYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HG22	1:A:37:VAL:N	2.33	0.42
1:A:48:MET:O	1:A:51:ASP:HB2	2.20	0.42
1:A:79:PHE:CE1	1:A:86:VAL:HG11	2.55	0.42
1:A:132:VAL:O	1:A:132:VAL:HG23	2.19	0.41
1:A:393:MET:CE	1:A:396:LYS:HD3	2.50	0.41
1:A:186:VAL:CG2	1:A:187:ALA:N	2.83	0.41
1:A:380:VAL:HG12	1:A:380:VAL:O	2.20	0.41
1:A:48:MET:HE3	1:A:151:ARG:NE	2.35	0.41
1:A:147:GLY:HA3	1:A:223:TYR:CE1	2.56	0.41
1:A:89:ALA:HB2	1:A:112:ALA:HB3	2.02	0.41
1:A:153:LYS:CG	1:A:214:GLN:HE21	2.34	0.41
1:A:232:LYS:CB	1:A:232:LYS:NZ	2.84	0.41
1:A:284:TYR:O	1:A:288:VAL:HG23	2.21	0.41
1:A:360:ALA:O	1:A:364:MET:HE2	2.20	0.41
1:A:416:PHE:O	1:A:419:GLN:N	2.47	0.41
1:A:260:ASP:C	1:A:260:ASP:OD2	2.60	0.40
1:A:88:LYS:HB2	1:A:112:ALA:HB1	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:OE1	1:A:346:LEU:CD2 2_664	2.12	0.08

## 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	367/457 (80%)	318 (87%)	34 (9%)	15 (4%)	<b>3</b> <b>9</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	124	SER
1	A	29	LYS
1	A	31	ARG
1	A	114	GLY
1	A	126	ALA
1	A	145	ASP
1	A	155	ARG
1	A	385	LYS
1	A	86	VAL
1	A	87	ILE
1	A	123	PRO
1	A	387	ALA
1	A	117	GLY
1	A	120	PRO

### 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	308/376 (82%)	288 (94%)	20 (6%)	<b>17</b> 44

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	51	ASP
1	A	57	TYR
1	A	78	VAL
1	A	79	PHE
1	A	107	CYS
1	A	119	LEU
1	A	123	PRO
1	A	159	TYR
1	A	186	VAL
1	A	189	THR
1	A	251	GLU

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Mol	Chain	Res	Type
1	A	256	SER
1	A	286	GLN
1	A	366	GLU
1	A	376	LYS
1	A	381	ASN
1	A	384	ASN
1	A	389	LEU
1	A	392	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	196	HIS
1	A	210	GLN
1	A	214	GLN
1	A	361	GLN
1	A	381	ASN
1	A	384	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

2 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
2	SO4	A	601	-	4,4,4	0.40	0	6,6,6	0.22	0
2	SO4	A	602	-	4,4,4	0.38	0	6,6,6	0.26	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SO4	1	0

## 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, 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	374/457 (81%)	-0.08	10 (2%) 54 44	23, 47, 81, 96	17 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ALA	4.5
1	A	128	LEU	4.3
1	A	58	ASN	3.2
1	A	107	CYS	2.9
1	A	106	LEU	2.9
1	A	59	GLY	2.7
1	A	129	PHE	2.6
1	A	127	THR	2.4
1	A	33	VAL	2.4
1	A	105	LEU	2.1

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	601	5/5	0.96	0.13	65,66,71,72	0
2	SO4	A	602	5/5	0.97	0.12	53,58,63,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.