



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:48 PM GMT

PDB ID : 3O2M  
Title : Crystal Structure of JNK1-alpha1 isoform complex with a biaryl tetrazol (A-82118)  
Authors : Abad-Zapatero, C.  
Deposited on : 2010-07-22  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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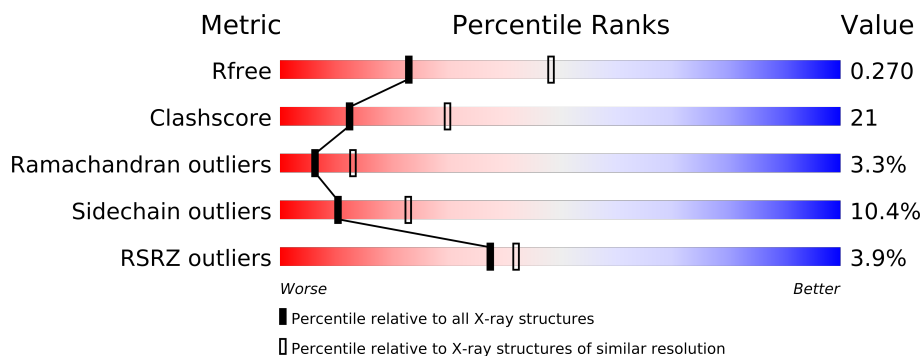
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	370	
1	B	370	
2	F	10	
2	G	10	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	46A	B	701	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6037 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2894	1853	488	531	22			
1	B	358	Total	C	N	O	S	0	0	0
			2894	1853	488	531	22			

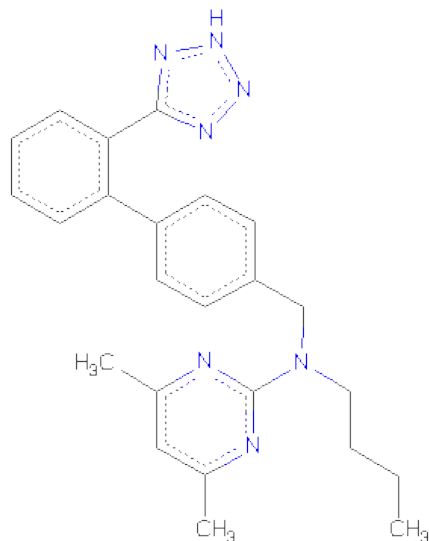
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	ENGINEERED MUTATION	UNP P45983
A	185	GLU	TYR	ENGINEERED MUTATION	UNP P45983
A	208	ILE	LEU	VARIANT	UNP P45983
A	247	ALA	GLU	SEE REMARK 999	UNP P45983
A	258	ASN	THR	SEE REMARK 999	UNP P45983
A	365	HIS	-	EXPRESSION TAG	UNP P45983
A	366	HIS	-	EXPRESSION TAG	UNP P45983
A	367	HIS	-	EXPRESSION TAG	UNP P45983
A	368	HIS	-	EXPRESSION TAG	UNP P45983
A	369	HIS	-	EXPRESSION TAG	UNP P45983
A	370	HIS	-	EXPRESSION TAG	UNP P45983
B	183	GLU	THR	ENGINEERED MUTATION	UNP P45983
B	185	GLU	TYR	ENGINEERED MUTATION	UNP P45983
B	208	ILE	LEU	VARIANT	UNP P45983
B	247	ALA	GLU	SEE REMARK 999	UNP P45983
B	258	ASN	THR	SEE REMARK 999	UNP P45983
B	365	HIS	-	EXPRESSION TAG	UNP P45983
B	366	HIS	-	EXPRESSION TAG	UNP P45983
B	367	HIS	-	EXPRESSION TAG	UNP P45983
B	368	HIS	-	EXPRESSION TAG	UNP P45983
B	369	HIS	-	EXPRESSION TAG	UNP P45983
B	370	HIS	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is a protein called C-Jun-amino-terminal kinase-interacting protein 1, JIP1, 10MER PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			83	55	15	13			
2	G	10	Total	C	N	O	0	0	0
			84	55	15	14			

- Molecule 3 is N-BUTYL-4,6-DIMETHYL-N-{[2'-(2H-TETRAZOL-5-YL)BIPHENYL-4-YL] METHYL}PYRIMIDIN-2-AMINE (three-letter code: 46A) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			31	24	7		
3	B	1	Total	C	N	0	0
			31	24	7		

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



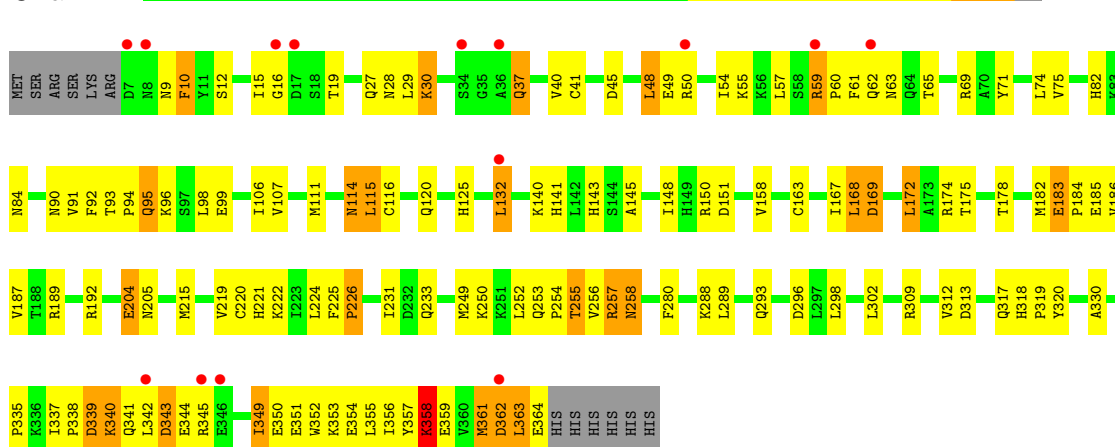
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

### 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 errors 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.

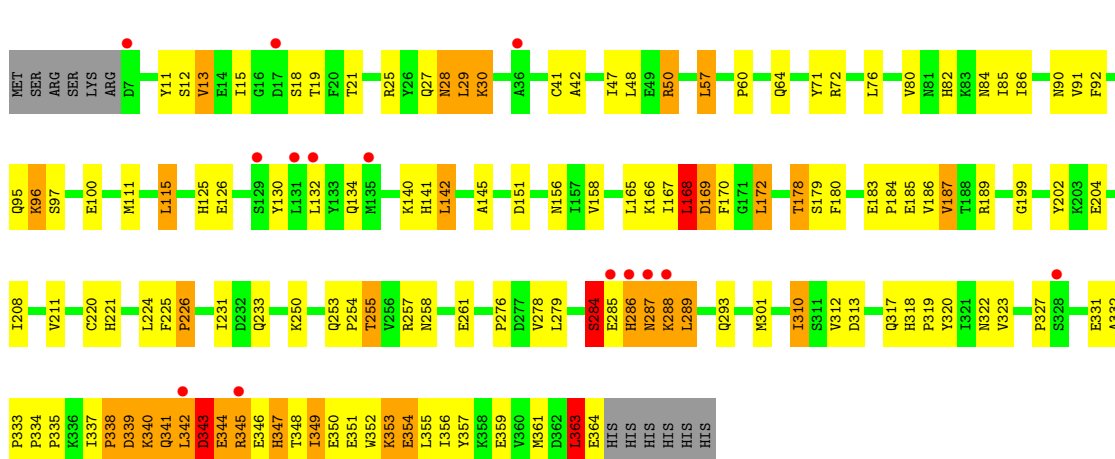
- Molecule 1: Mitogen-activated protein kinase 8

Chain A:



- Molecule 1: Mitogen-activated protein kinase 8

Chain B:



- Molecule 2: C-Jun-amino-terminal kinase-interacting protein 1, JIP1, 10MER PEPTIDE

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.38Å 158.38Å 123.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.70 19.88 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.5 (19.88-2.70) 93.7 (19.88-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.71Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.233 , 0.266 0.235 , 0.270	Depositor DCC
$R_{free}$ test set	4681 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.1	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49653 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 46A, 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	0.61	0/2959	0.76	0/4002
1	B	0.59	0/2959	0.77	2/4002 (0.0%)
2	F	0.68	0/85	0.76	0/114
2	G	0.81	0/86	0.75	0/114
All	All	0.60	0/6089	0.77	2/8232 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	LEU	CA-CB-CG	6.56	130.39	115.30
1	B	363	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2894	0	2904	112	0
1	B	2894	0	2904	137	0
2	F	83	0	91	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	84	0	91	3	0
3	A	31	0	27	2	0
3	B	31	0	27	5	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
All	All	6037	0	6044	256	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (256) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:ARG:HD2	1:A:62:GLN:HB3	1.29	1.15
1:A:168:LEU:HD22	1:A:169:ASP:N	1.75	1.01
1:B:250:LYS:HG3	1:B:257:ARG:HH21	1.29	0.98
1:B:13:VAL:HG21	1:B:29:LEU:HG	1.55	0.87
1:B:332:ALA:HB1	1:B:333:PRO:HD2	1.55	0.87
1:A:250:LYS:HD2	1:A:257:ARG:HH22	1.41	0.85
1:B:288:LYS:HD2	1:B:323:VAL:HG12	1.58	0.85
1:A:168:LEU:HD22	1:A:169:ASP:H	1.39	0.84
1:A:94:PRO:HG2	1:A:95:GLN:HE22	1.40	0.84
1:B:91:VAL:HG11	1:B:363:LEU:HG	1.60	0.83
1:B:96:LYS:HD3	1:B:100:GLU:OE1	1.80	0.81
1:B:342:LEU:C	1:B:344:GLU:H	1.83	0.80
1:B:341:GLN:HA	1:B:341:GLN:HE21	1.48	0.78
1:B:168:LEU:HD22	1:B:169:ASP:N	1.98	0.77
1:A:352:TRP:O	1:A:356:ILE:HG12	1.86	0.76
1:B:76:LEU:O	1:B:80:VAL:HG23	1.85	0.76
2:F:555:LYS:HD2	2:F:556:ARG:H	1.51	0.75
1:A:231:ILE:HG12	3:A:701:46A:H2	1.66	0.75
1:B:287:ASN:CG	1:B:288:LYS:H	1.89	0.74
1:B:342:LEU:O	1:B:344:GLU:N	2.20	0.74
1:B:82:HIS:HD2	1:B:84:ASN:H	1.33	0.73
1:A:185:GLU:HG2	1:B:254:PRO:HB2	1.69	0.73
2:F:561:ASN:ND2	2:F:563:PHE:H	1.88	0.72
1:A:59:ARG:HH11	1:A:59:ARG:HG3	1.55	0.71
1:A:29:LEU:O	1:A:30:LYS:HB3	1.91	0.70
1:B:351:GLU:O	1:B:354:GLU:HB3	1.92	0.69
1:A:94:PRO:HG2	1:A:95:GLN:NE2	2.07	0.69
1:A:250:LYS:HD2	1:A:257:ARG:NH2	2.07	0.69
1:A:65:THR:O	1:A:69:ARG:HG3	1.94	0.67
1:B:340:LYS:O	1:B:343:ASP:HB2	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.61	0.66
1:B:72:ARG:HH21	1:B:172:LEU:HA	1.61	0.66
1:B:13:VAL:HG21	1:B:29:LEU:CG	2.24	0.66
1:B:50:ARG:HG2	1:B:50:ARG:NH1	2.10	0.65
1:B:183:GLU:O	1:B:186:VAL:HG12	1.95	0.65
1:A:359:GLU:O	1:A:363:LEU:HB2	1.96	0.65
1:B:125:HIS:HB3	1:B:289:LEU:HB3	1.79	0.65
1:B:287:ASN:HD21	1:B:288:LYS:HE3	1.61	0.64
1:A:225:PHE:O	1:A:226:PRO:O	2.15	0.64
1:B:318:HIS:HD2	1:B:320:TYR:H	1.44	0.64
1:A:150:ARG:HH21	1:A:174:ARG:HD3	1.62	0.64
1:A:340:LYS:O	1:A:343:ASP:HB3	1.98	0.63
1:A:338:PRO:O	1:A:339:ASP:HB3	1.98	0.63
1:B:13:VAL:CG2	1:B:29:LEU:HG	2.27	0.62
1:B:357:TYR:O	1:B:361:MET:HG2	1.98	0.62
1:A:82:HIS:HD2	1:A:84:ASN:H	1.46	0.62
2:F:561:ASN:HD22	2:F:563:PHE:H	1.46	0.62
1:B:338:PRO:O	1:B:339:ASP:HB2	1.99	0.62
1:B:12:SER:HB3	1:B:21:THR:HA	1.82	0.62
1:B:355:LEU:H	1:B:355:LEU:HD12	1.65	0.62
1:B:71:TYR:OH	1:B:340:LYS:HB2	2.00	0.61
1:A:27:GLN:O	1:A:28:ASN:HB2	2.00	0.61
1:B:287:ASN:CG	1:B:288:LYS:N	2.53	0.61
1:B:80:VAL:HG11	1:B:142:LEU:HD11	1.81	0.61
1:B:349:ILE:HG13	1:B:350:GLU:H	1.66	0.61
1:B:189:ARG:HD3	4:B:801:SO4:O1	2.00	0.61
1:B:208:ILE:HG21	1:B:310:ILE:HG22	1.83	0.60
1:B:337:ILE:HG21	1:B:341:GLN:HB2	1.83	0.60
1:B:363:LEU:O	1:B:363:LEU:HD12	2.01	0.60
1:B:351:GLU:O	1:B:355:LEU:HD12	2.02	0.60
1:B:225:PHE:O	1:B:226:PRO:O	2.19	0.60
1:B:250:LYS:HA	1:B:257:ARG:HE	1.67	0.60
1:B:29:LEU:O	1:B:42:ALA:O	2.20	0.60
1:B:342:LEU:C	1:B:344:GLU:N	2.55	0.60
1:B:82:HIS:CD2	1:B:84:ASN:H	2.19	0.59
1:A:148:ILE:HG12	1:A:204:GLU:HA	1.84	0.59
2:G:561:ASN:HD21	2:G:563:PHE:HB2	1.67	0.59
1:A:258:ASN:HD22	1:A:258:ASN:C	2.06	0.59
1:B:11:TYR:OH	1:B:27:GLN:HA	2.03	0.58
1:A:351:GLU:O	1:A:354:GLU:HB3	2.03	0.58
1:B:95:GLN:HG2	1:B:100:GLU:O	2.02	0.58
1:A:183:GLU:HA	1:A:185:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:313:ASP:O	1:B:317:GLN:HG2	2.04	0.58
1:A:40:VAL:HG22	1:A:55:LYS:HB2	1.86	0.58
1:A:60:PRO:HB2	1:A:61:PHE:CE1	2.39	0.58
1:B:343:ASP:O	1:B:345:ARG:N	2.32	0.57
2:F:561:ASN:C	2:F:561:ASN:HD22	2.06	0.57
1:B:180:PHE:HB2	3:B:701:46A:N21	2.20	0.57
1:B:286:HIS:N	1:B:286:HIS:CD2	2.73	0.57
1:A:318:HIS:HD2	1:A:320:TYR:H	1.51	0.57
1:A:151:ASP:HB2	1:A:172:LEU:HD23	1.86	0.56
1:B:231:ILE:HG12	3:B:701:46A:H2	1.87	0.56
1:B:289:LEU:HD13	1:B:289:LEU:N	2.19	0.56
1:B:233:GLN:NE2	1:B:233:GLN:HA	2.21	0.56
1:A:71:TYR:CZ	1:A:355:LEU:HD23	2.41	0.56
1:A:10:PHE:N	1:A:10:PHE:CD1	2.74	0.56
1:B:178:THR:O	1:B:202:TYR:HE2	1.88	0.55
1:B:332:ALA:HB1	1:B:333:PRO:CD	2.34	0.55
1:A:349:ILE:HG12	1:A:350:GLU:H	1.72	0.55
1:A:296:ASP:OD2	1:A:318:HIS:HE1	1.89	0.55
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.41	0.55
1:B:50:ARG:CG	1:B:50:ARG:HH11	2.19	0.55
1:A:358:LYS:HG3	1:A:359:GLU:N	2.22	0.55
1:A:357:TYR:O	1:A:361:MET:HG2	2.06	0.55
1:B:140:LYS:HB2	1:B:312:VAL:HG11	1.90	0.54
1:B:29:LEU:N	1:B:29:LEU:HD22	2.22	0.54
1:B:142:LEU:HD21	1:B:170:PHE:CE2	2.43	0.54
1:A:358:LYS:HG3	1:A:362:ASP:OD1	2.08	0.53
1:B:345:ARG:HH11	1:B:345:ARG:HB2	1.74	0.53
1:B:19:THR:HG22	1:B:19:THR:O	2.07	0.53
1:B:339:ASP:OD1	1:B:342:LEU:HB2	2.09	0.53
1:A:255:THR:HB	3:B:701:46A:H28	1.91	0.53
1:A:59:ARG:CG	1:A:59:ARG:HH11	2.20	0.53
1:A:205:ASN:ND2	1:A:309:ARG:HB3	2.24	0.53
1:A:254:PRO:HB2	1:B:185:GLU:HG2	1.90	0.52
1:A:256:VAL:HG22	3:B:701:46A:H29B	1.91	0.52
1:A:111:MET:HG3	1:A:158:VAL:CG2	2.39	0.52
1:B:287:ASN:ND2	1:B:288:LYS:HE3	2.25	0.52
1:B:343:ASP:C	1:B:345:ARG:H	2.11	0.52
1:B:183:GLU:N	1:B:184:PRO:HD3	2.25	0.52
1:B:318:HIS:CD2	1:B:320:TYR:H	2.27	0.52
1:A:74:LEU:CD1	1:A:106:ILE:HD11	2.39	0.52
1:B:80:VAL:HG11	1:B:142:LEU:CD1	2.40	0.52
1:B:286:HIS:O	1:B:288:LYS:N	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:LEU:HD22	1:B:169:ASP:H	1.75	0.51
1:A:37:GLN:OE1	1:A:37:GLN:N	2.43	0.51
1:B:15:ILE:HD11	1:B:29:LEU:HB3	1.92	0.51
1:B:359:GLU:OE1	1:B:359:GLU:HA	2.11	0.51
1:B:347:HIS:ND1	1:B:347:HIS:N	2.59	0.51
1:B:317:GLN:HA	1:B:322:ASN:HD22	1.76	0.51
1:A:111:MET:HG3	1:A:158:VAL:HG23	1.93	0.51
1:B:250:LYS:HG3	1:B:257:ARG:NH2	2.11	0.51
1:B:211:VAL:HB	1:B:301:MET:HE2	1.93	0.50
1:A:98:LEU:O	1:A:353:LYS:HE2	2.11	0.50
1:B:340:LYS:H	1:B:340:LYS:CD	2.23	0.50
1:A:75:VAL:HG22	1:A:340:LYS:HE3	1.93	0.50
1:A:62:GLN:O	1:A:63:ASN:HB3	2.12	0.50
1:A:150:ARG:HH21	1:A:174:ARG:CD	2.24	0.50
1:B:224:LEU:HD23	1:B:225:PHE:CE2	2.47	0.50
1:A:249:MET:O	1:A:257:ARG:HG3	2.10	0.50
1:B:257:ARG:O	1:B:261:GLU:HG3	2.12	0.50
1:B:359:GLU:O	1:B:363:LEU:HB2	2.12	0.49
1:A:54:ILE:HG12	1:A:107:VAL:HG22	1.93	0.49
1:B:341:GLN:O	1:B:344:GLU:HG2	2.12	0.49
1:B:341:GLN:HA	1:B:341:GLN:NE2	2.23	0.49
1:B:184:PRO:O	1:B:187:VAL:HG13	2.12	0.49
1:A:343:ASP:C	1:A:345:ARG:H	2.16	0.49
1:A:293:GLN:HE21	1:A:319:PRO:HB2	1.76	0.49
1:A:358:LYS:O	1:A:359:GLU:C	2.51	0.49
1:A:145:ALA:HB2	1:A:335:PRO:HG2	1.95	0.49
1:B:15:ILE:HD12	1:B:41:CYS:SG	2.52	0.49
1:B:338:PRO:HD2	1:B:340:LYS:HD3	1.95	0.49
2:F:555:LYS:HD2	2:F:556:ARG:N	2.22	0.49
1:A:82:HIS:CD2	1:A:84:ASN:H	2.29	0.49
1:B:145:ALA:HB2	1:B:335:PRO:HG2	1.95	0.48
1:A:184:PRO:HD2	3:B:701:46A:H14	1.95	0.48
1:B:359:GLU:O	1:B:363:LEU:CB	2.61	0.48
1:B:340:LYS:H	1:B:340:LYS:HD2	1.77	0.48
1:A:220:CYS:O	1:A:221:HIS:HB2	2.14	0.48
1:B:25:ARG:NH2	1:B:48:LEU:HD13	2.29	0.48
1:B:92:PHE:CD1	1:B:92:PHE:C	2.87	0.48
1:B:11:TYR:OH	1:B:29:LEU:HD21	2.14	0.48
1:A:288:LYS:HG3	1:A:319:PRO:O	2.14	0.48
1:A:183:GLU:N	1:A:184:PRO:HD3	2.29	0.48
1:A:318:HIS:CD2	1:A:320:TYR:H	2.31	0.48
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.68	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ASP:O	1:A:49:GLU:N	2.43	0.47
1:A:341:GLN:C	1:A:343:ASP:N	2.68	0.47
1:A:338:PRO:O	1:A:339:ASP:CB	2.62	0.47
1:B:276:PRO:HD2	1:B:279:LEU:HD12	1.97	0.47
1:A:358:LYS:CG	1:A:359:GLU:N	2.77	0.46
1:A:349:ILE:HG12	1:A:350:GLU:N	2.30	0.46
1:A:215:MET:SD	1:A:298:LEU:HG	2.56	0.46
1:A:19:THR:HG22	1:A:19:THR:O	2.14	0.46
1:A:15:ILE:HD11	1:A:29:LEU:HB3	1.97	0.46
1:B:348:THR:O	1:B:349:ILE:C	2.52	0.46
1:B:156:ASN:O	1:B:168:LEU:HD12	2.16	0.46
1:A:59:ARG:NH1	1:A:59:ARG:CG	2.78	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.90	0.46
1:A:9:ASN:ND2	1:A:9:ASN:N	2.63	0.46
1:B:82:HIS:HB2	1:B:141:HIS:CD2	2.51	0.45
1:B:156:ASN:HA	1:B:168:LEU:CD1	2.46	0.45
1:B:317:GLN:HA	1:B:317:GLN:NE2	2.31	0.45
2:G:555:LYS:HA	2:G:555:LYS:HD2	1.61	0.45
1:A:252:LEU:HB2	1:A:257:ARG:HB2	1.97	0.45
1:B:111:MET:HG3	1:B:158:VAL:CG2	2.46	0.45
1:B:220:CYS:O	1:B:221:HIS:HB2	2.16	0.45
1:A:140:LYS:NZ	1:A:330:ALA:O	2.48	0.45
1:B:85:ILE:HG23	1:B:170:PHE:HZ	1.82	0.45
1:A:313:ASP:O	1:A:317:GLN:HG2	2.16	0.45
1:A:40:VAL:HA	1:A:54:ILE:O	2.17	0.45
1:A:74:LEU:HD12	1:A:106:ILE:HD11	1.99	0.45
1:B:286:HIS:O	1:B:287:ASN:C	2.54	0.45
2:F:561:ASN:C	2:F:561:ASN:ND2	2.71	0.44
1:B:333:PRO:HA	1:B:334:PRO:HD2	1.69	0.44
1:A:125:HIS:HB3	1:A:289:LEU:HB3	1.99	0.44
3:A:701:46A:H28	1:B:255:THR:HB	1.99	0.44
1:A:341:GLN:C	1:A:343:ASP:H	2.20	0.44
1:B:27:GLN:O	1:B:28:ASN:HB2	2.16	0.44
1:B:72:ARG:NH2	1:B:172:LEU:HA	2.30	0.44
1:B:348:THR:O	1:B:351:GLU:HB2	2.17	0.44
1:A:349:ILE:CG1	1:A:350:GLU:N	2.81	0.44
1:A:184:PRO:HD2	1:A:185:GLU:OE2	2.16	0.44
1:B:345:ARG:O	1:B:346:GLU:HG3	2.18	0.44
1:B:151:ASP:O	1:B:156:ASN:ND2	2.48	0.44
1:B:348:THR:OG1	1:B:351:GLU:HG3	2.18	0.44
1:A:222:LYS:HE2	1:A:222:LYS:HB3	1.81	0.44
1:A:168:LEU:O	1:A:169:ASP:CB	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:PRO:HB2	1:B:185:GLU:CG	2.47	0.43
1:A:343:ASP:CG	1:A:343:ASP:O	2.56	0.43
2:G:562:LEU:O	2:G:563:PHE:HD2	2.02	0.43
1:B:86:ILE:HD12	1:B:166:LYS:HD3	2.01	0.43
1:A:340:LYS:HG2	1:A:340:LYS:H	1.45	0.43
1:B:130:TYR:CE2	1:B:134:GLN:NE2	2.87	0.43
1:B:179:SER:OG	1:B:199:GLY:HA2	2.19	0.43
1:B:284:SER:HB2	1:B:285:GLU:H	1.49	0.43
1:A:15:ILE:HG21	1:A:41:CYS:SG	2.58	0.43
1:A:358:LYS:O	1:A:361:MET:N	2.51	0.43
1:A:341:GLN:O	1:A:344:GLU:HG2	2.18	0.43
1:B:233:GLN:HA	1:B:233:GLN:HE21	1.84	0.43
1:B:97:SER:HA	1:B:357:TYR:OH	2.18	0.43
1:A:40:VAL:HG22	1:A:55:LYS:CB	2.48	0.43
1:A:337:ILE:HA	1:A:338:PRO:HD3	1.92	0.43
1:B:71:TYR:HB2	1:B:356:ILE:HD11	2.00	0.43
1:B:350:GLU:OE1	1:B:353:LYS:HD3	2.19	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.75	0.42
1:A:10:PHE:HD1	1:A:10:PHE:N	2.14	0.42
1:A:132:LEU:HD21	1:A:215:MET:HG3	2.00	0.42
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.80	0.42
1:A:29:LEU:O	1:A:30:LYS:CB	2.63	0.42
1:B:288:LYS:HB3	1:B:289:LEU:HD13	2.02	0.42
1:A:48:LEU:HD23	1:A:50:ARG:HE	1.83	0.42
1:B:64:GLN:NE2	1:B:347:HIS:O	2.52	0.42
1:A:338:PRO:HB2	1:A:340:LYS:CD	2.50	0.42
1:B:57:LEU:HB3	1:B:60:PRO:HG3	2.01	0.42
1:A:143:HIS:ND1	1:A:312:VAL:HG21	2.34	0.42
1:B:288:LYS:O	1:B:293:GLN:OE1	2.38	0.42
1:B:361:MET:C	1:B:363:LEU:H	2.23	0.42
1:B:28:ASN:C	1:B:29:LEU:HD22	2.40	0.42
1:B:318:HIS:HA	1:B:319:PRO:HD3	1.97	0.42
1:A:289:LEU:N	1:A:289:LEU:CD1	2.82	0.42
1:B:318:HIS:CD2	1:B:319:PRO:HD2	2.54	0.42
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.83	0.42
1:B:29:LEU:O	1:B:30:LYS:O	2.37	0.41
2:F:556:ARG:HA	2:F:557:PRO:HD3	1.92	0.41
1:A:114:ASN:HB3	1:A:116:CYS:H	1.85	0.41
1:A:189:ARG:HB3	1:A:192:ARG:NH2	2.35	0.41
1:B:286:HIS:N	1:B:286:HIS:HD2	2.17	0.41
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.64	0.41
1:B:349:ILE:O	1:B:350:GLU:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:GLN:NE2	1:A:169:ASP:OD2	2.54	0.41
1:B:352:TRP:O	1:B:354:GLU:N	2.54	0.41
1:A:167:ILE:HG22	1:A:168:LEU:N	2.36	0.41
1:B:167:ILE:HG22	1:B:168:LEU:N	2.35	0.41
1:A:183:GLU:O	1:A:186:VAL:HG12	2.21	0.41
1:B:86:ILE:HD12	1:B:86:ILE:HA	1.79	0.41
1:A:233:GLN:NE2	1:A:233:GLN:HA	2.36	0.41
1:B:25:ARG:HH21	1:B:48:LEU:HD13	1.85	0.41
1:A:90:ASN:ND2	1:A:91:VAL:H	2.19	0.41
1:B:342:LEU:O	1:B:342:LEU:HD22	2.21	0.40
1:A:71:TYR:O	1:A:75:VAL:HG23	2.21	0.40
1:A:219:VAL:HG21	1:A:280:PHE:CE1	2.56	0.40
1:A:9:ASN:N	1:A:9:ASN:HD22	2.20	0.40
1:B:71:TYR:HD1	1:B:356:ILE:HD13	1.86	0.40
1:B:347:HIS:HB3	1:B:351:GLU:CD	2.42	0.40
1:A:192:ARG:NH2	4:A:801:SO4:O1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	356/370 (96%)	313 (88%)	35 (10%)	8 (2%)	10	25
1	B	356/370 (96%)	310 (87%)	30 (8%)	16 (4%)	4	7
2	F	8/10 (80%)	8 (100%)	0	0	100	100
2	G	8/10 (80%)	8 (100%)	0	0	100	100
All	All	728/760 (96%)	639 (88%)	65 (9%)	24 (3%)	6	13

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	PRO
1	A	339	ASP

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Mol	Chain	Res	Type
1	B	226	PRO
1	B	287	ASN
1	B	288	LYS
1	B	339	ASP
1	B	343	ASP
1	B	344	GLU
1	A	16	GLY
1	A	362	ASP
1	B	349	ILE
1	A	358	LYS
1	B	29	LEU
1	B	30	LYS
1	B	331	GLU
1	A	30	LYS
1	B	284	SER
1	B	338	PRO
1	A	169	ASP
1	A	361	MET
1	B	169	ASP
1	B	353	LYS
1	B	47	ILE
1	B	327	PRO

### 5.3.2 Protein sidechains ⓘ

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	321/333 (96%)	287 (89%)	34 (11%)	10	22
1	B	321/333 (96%)	287 (89%)	34 (11%)	10	22
2	F	10/10 (100%)	9 (90%)	1 (10%)	11	25
2	G	10/10 (100%)	10 (100%)	0	100	100
All	All	662/686 (96%)	593 (90%)	69 (10%)	10	23

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	12	SER
1	A	37	GLN
1	A	48	LEU
1	A	57	LEU
1	A	59	ARG
1	A	93	THR
1	A	95	GLN
1	A	96	LYS
1	A	99	GLU
1	A	114	ASN
1	A	115	LEU
1	A	120	GLN
1	A	132	LEU
1	A	163	CYS
1	A	168	LEU
1	A	172	LEU
1	A	175	THR
1	A	178	THR
1	A	182	MET
1	A	183	GLU
1	A	187	VAL
1	A	204	GLU
1	A	253	GLN
1	A	255	THR
1	A	257	ARG
1	A	258	ASN
1	A	340	LYS
1	A	342	LEU
1	A	343	ASP
1	A	349	ILE
1	A	358	LYS
1	A	363	LEU
1	A	364	GLU
2	F	561	ASN
1	B	13	VAL
1	B	18	SER
1	B	28	ASN
1	B	50	ARG
1	B	57	LEU
1	B	90	ASN
1	B	96	LYS
1	B	115	LEU

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Mol	Chain	Res	Type
1	B	126	GLU
1	B	132	LEU
1	B	142	LEU
1	B	165	LEU
1	B	168	LEU
1	B	172	LEU
1	B	178	THR
1	B	187	VAL
1	B	204	GLU
1	B	253	GLN
1	B	255	THR
1	B	258	ASN
1	B	278	VAL
1	B	284	SER
1	B	286	HIS
1	B	289	LEU
1	B	310	ILE
1	B	340	LYS
1	B	341	GLN
1	B	342	LEU
1	B	343	ASP
1	B	345	ARG
1	B	347	HIS
1	B	354	GLU
1	B	363	LEU
1	B	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	27	GLN
1	A	82	HIS
1	A	90	ASN
1	A	95	GLN
1	A	114	ASN
1	A	141	HIS
1	A	235	ASN
1	A	240	GLN
1	A	253	GLN
1	A	258	ASN
1	A	293	GLN

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Mol	Chain	Res	Type
1	A	317	GLN
1	A	318	HIS
1	A	341	GLN
2	F	561	ASN
1	B	9	ASN
1	B	37	GLN
1	B	62	GLN
1	B	82	HIS
1	B	90	ASN
1	B	141	HIS
1	B	233	GLN
1	B	235	ASN
1	B	253	GLN
1	B	258	ASN
1	B	287	ASN
1	B	317	GLN
1	B	318	HIS
1	B	322	ASN
1	B	341	GLN
2	G	561	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	$\# Z  > 2$
3	46A	A	701	-	34,34,34	1.74	3 (8%)	44,46,46	1.79	10 (22%)
4	SO4	A	801	-	4,4,4	1.55	0	6,6,6	0.24	0
4	SO4	A	802	-	4,4,4	0.46	0	6,6,6	0.18	0
3	46A	B	701	-	34,34,34	1.75	4 (11%)	44,46,46	1.95	11 (25%)
4	SO4	B	801	-	4,4,4	1.76	1 (25%)	6,6,6	0.18	0
4	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.15	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	46A	A	701	-	-	0/20/20/20	0/4/4/4
4	SO4	A	801	-	-	0/0/0/0	0/0/0/0
4	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	46A	B	701	-	-	0/20/20/20	0/4/4/4
4	SO4	B	801	-	-	0/0/0/0	0/0/0/0
4	SO4	B	802	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	46A	C12-C17	7.79	1.53	1.41
3	B	701	46A	C12-C17	7.30	1.52	1.41
3	B	701	46A	N19-N20	2.85	1.37	1.34
3	A	701	46A	C18-N22	2.59	1.36	1.33
3	B	701	46A	C18-N22	2.21	1.36	1.33
4	B	801	SO4	O3-S	-2.12	1.40	1.47
3	B	701	46A	C25-N	2.10	1.39	1.35
3	A	701	46A	C11-C10	2.10	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	46A	N22-C18-N19	-7.57	107.07	112.01
3	A	701	46A	N22-C18-N19	-5.57	108.38	112.01
3	B	701	46A	C18-N19-N20	4.79	109.13	105.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	46A	C25-N2-C27	4.09	119.13	115.20
3	B	701	46A	C25-N2-C27	3.74	118.80	115.20
3	A	701	46A	C18-N19-N20	3.71	108.28	105.34
3	B	701	46A	C18-N22-N21	3.69	109.59	104.17
3	A	701	46A	C6-C5-N	3.66	119.90	114.44
3	B	701	46A	C25-N1-C23	3.46	118.53	115.20
3	B	701	46A	C6-C5-N	3.32	119.40	114.44
3	A	701	46A	C25-N1-C23	3.15	118.23	115.20
3	A	701	46A	C18-N22-N21	2.77	108.25	104.17
3	A	701	46A	C17-C18-N22	2.61	128.30	123.95
3	A	701	46A	C5-C6-C11	2.57	125.60	120.78
3	A	701	46A	C5-C6-C7	-2.56	115.97	120.78
3	B	701	46A	C17-C18-N22	2.27	127.73	123.95
3	A	701	46A	N2-C25-N	2.15	119.55	117.11
3	B	701	46A	C5-C6-C7	-2.06	116.91	120.78
3	B	701	46A	C5-C6-C11	2.05	124.62	120.78
3	B	701	46A	N2-C25-N1	-2.04	122.76	126.28
3	B	701	46A	N2-C25-N	2.02	119.40	117.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	358/370 (96%)	0.01	14 (3%) 37 42	31, 51, 95, 132	0
1	B	358/370 (96%)	0.03	14 (3%) 37 42	33, 54, 98, 135	0
2	F	10/10 (100%)	-0.16	0 100 100	40, 48, 70, 72	0
2	G	10/10 (100%)	-0.00	1 (10%) 8 8	48, 59, 72, 98	0
All	All	736/760 (96%)	0.02	29 (3%) 37 42	31, 53, 96, 135	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	6.4
1	A	7	ASP	6.1
1	B	288	LYS	5.8
1	B	345	ARG	3.9
1	B	7	ASP	3.9
1	A	59	ARG	3.5
1	A	345	ARG	3.4
1	B	131	LEU	3.3
1	A	16	GLY	3.2
2	G	563	PHE	3.1
1	A	36	ALA	3.1
1	A	346	GLU	2.9
1	A	34	SER	2.7
1	B	342	LEU	2.7
1	B	287	ASN	2.6
1	A	17	ASP	2.6
1	B	285	GLU	2.6
1	B	36	ALA	2.5
1	B	132	LEU	2.5
1	A	132	LEU	2.3
1	A	50	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	17	ASP	2.2
1	A	62	GLN	2.2
1	B	286	HIS	2.1
1	A	8	ASN	2.1
1	B	135	MET	2.1
1	B	129	SER	2.1
1	A	362	ASP	2.0
1	B	328	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	46A	B	701	31/31	0.30	3.02	53,53,53,53	0
3	46A	A	701	31/31	0.26	1.95	53,53,53,53	0
4	SO4	B	801	5/5	0.13	-0.49	53,53,53,53	0
4	SO4	A	801	5/5	0.12	-0.72	53,53,53,53	0
4	SO4	B	802	5/5	0.12	-1.36	53,53,53,53	0
4	SO4	A	802	5/5	0.10	-2.25	53,53,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.