



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:03 PM GMT

PDB ID : 1IHX  
Title : Crystal structure of two D-glyceraldehyde-3-phosphate dehydrogenase complexes: a case of asymmetry  
Authors : Shen, Y.-Q.; Song, S.-Y.; Lin, Z.-J.  
Deposited on : 2001-04-20  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

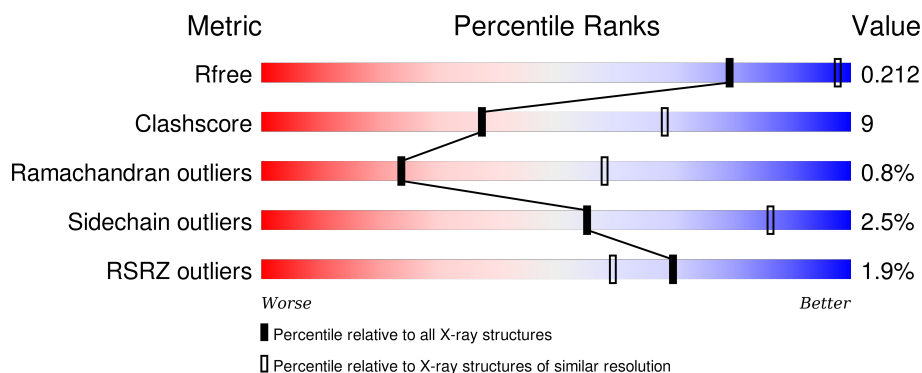
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	333	<div> <div>80%</div> <div>18%</div> <div>•</div> </div>
1	B	333	<div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	C	333	<div> <div>4%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
1	D	333	<div> <div>2%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>

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
2	SO4	A	501	-	-	-	X
2	SO4	B	506	-	X	-	-
2	SO4	C	503	-	-	-	X
2	SO4	C	507	-	X	-	-
2	SO4	D	504	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10476 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 GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2512	1593	421	482	16			
1	B	333	Total	C	N	O	S	0	0	0
			2512	1593	421	482	16			
1	C	333	Total	C	N	O	S	0	0	0
			2512	1593	421	482	16			
1	D	333	Total	C	N	O	S	0	0	0
			2512	1593	421	482	16			

There are 12 discrepancies between the modelled and reference sequences:

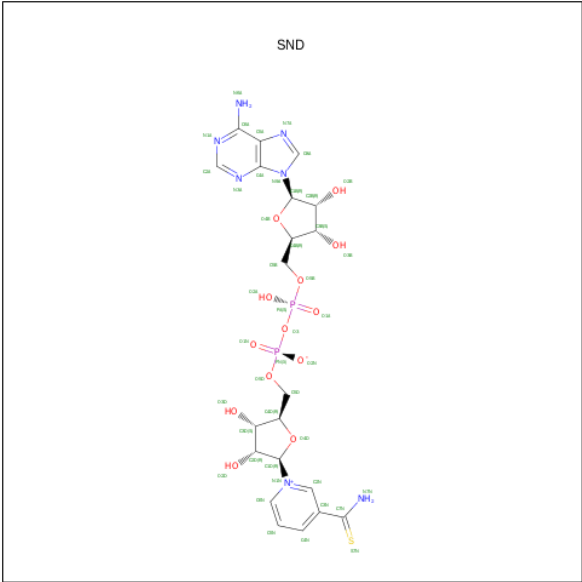
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	THR	ALA	SEE REMARK 999	UNP P56649
A	59	VAL	ALA	SEE REMARK 999	UNP P56649
A	261	THR	ALA	SEE REMARK 999	UNP P56649
B	18	THR	ALA	SEE REMARK 999	UNP P56649
B	59	VAL	ALA	SEE REMARK 999	UNP P56649
B	261	THR	ALA	SEE REMARK 999	UNP P56649
C	18	THR	ALA	SEE REMARK 999	UNP P56649
C	59	VAL	ALA	SEE REMARK 999	UNP P56649
C	261	THR	ALA	SEE REMARK 999	UNP P56649
D	18	THR	ALA	SEE REMARK 999	UNP P56649
D	59	VAL	ALA	SEE REMARK 999	UNP P56649
D	261	THR	ALA	SEE REMARK 999	UNP P56649

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



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

- Molecule 3 is THIONICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: SND) (formula:  $C_{21}H_{27}N_7O_{13}P_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
3	C	1	Total	C	N	O	P	S	0
			44	21	7	13	2	1	
3	D	1	Total	C	N	O	P	S	0
			44	21	7	13	2	1	

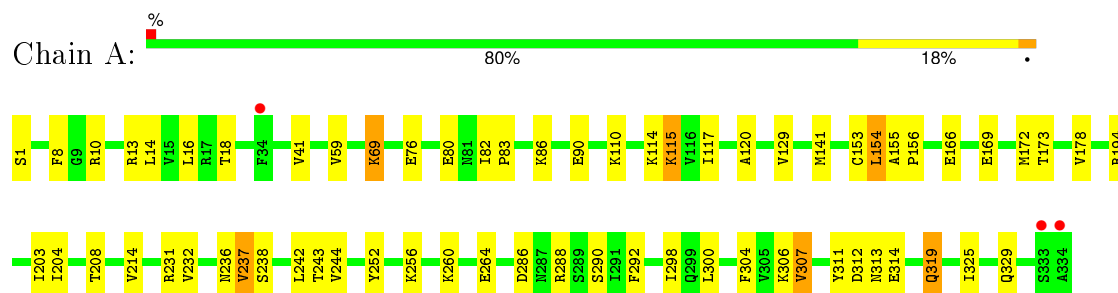
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	68	Total	O	0	0
			68	68		
4	C	50	Total	O	0	0
			50	50		
4	D	49	Total	O	0	0
			49	49		

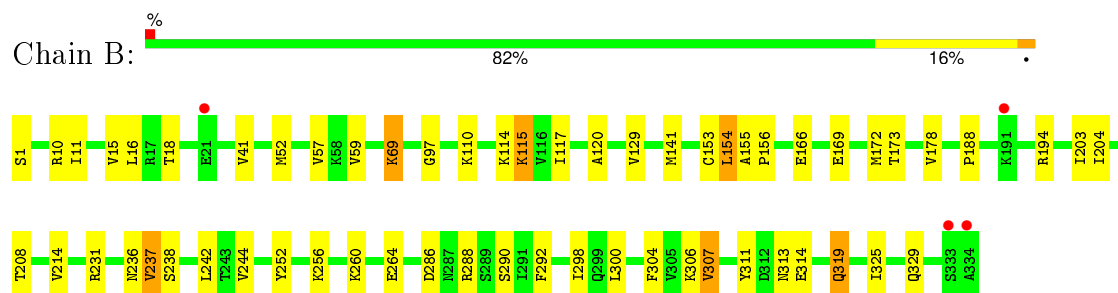
### 3 Residue-property plots [i](#)

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.

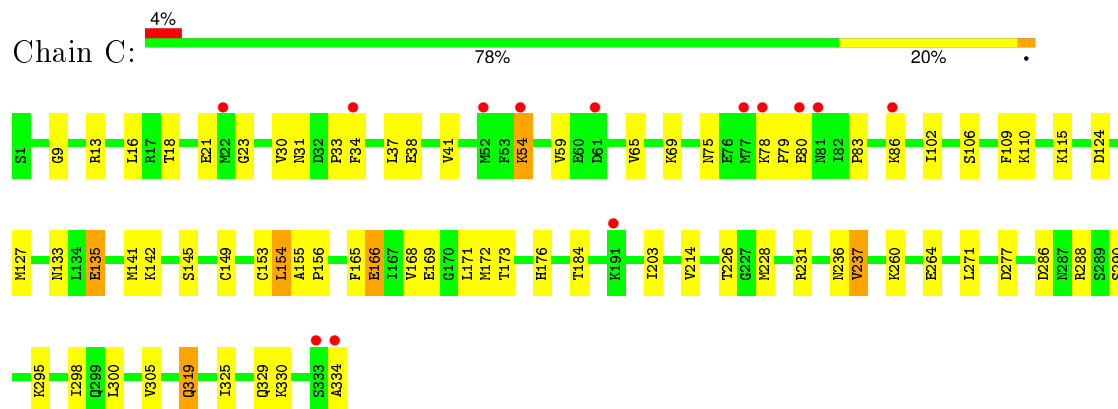
#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



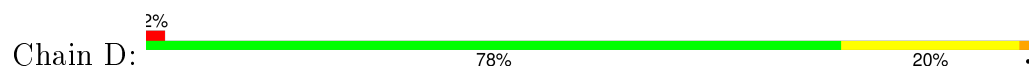
#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

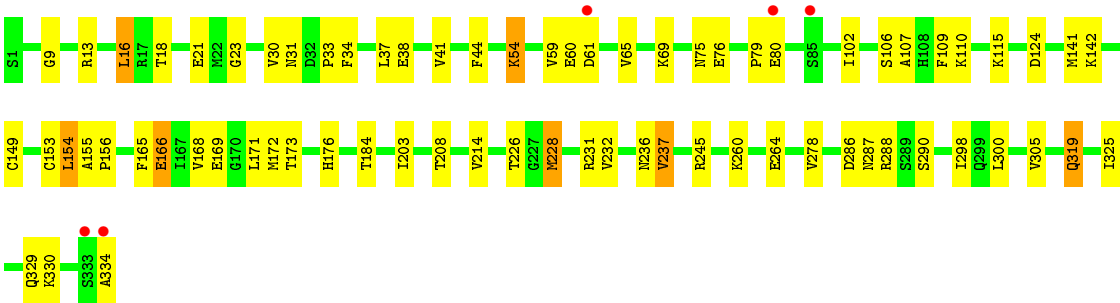


#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.41Å 100.51Å 128.44Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	29.84 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.84-2.80) 97.9 (29.84-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.80Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.177 , 0.204 0.187 , 0.212	Depositor DCC
$R_{free}$ test set	4424 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 44055 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SND, 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	0.45	0/2557	0.76	4/3455 (0.1%)
1	B	0.46	0/2557	0.75	4/3455 (0.1%)
1	C	0.42	0/2557	0.63	1/3455 (0.0%)
1	D	0.43	0/2557	0.64	1/3455 (0.0%)
All	All	0.44	0/10228	0.70	10/13820 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	B	10	ARG	NE-CZ-NH1	-12.53	114.04	120.30
1	A	10	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	B	10	ARG	NE-CZ-NH2	11.79	126.19	120.30
1	B	10	ARG	CD-NE-CZ	6.69	132.97	123.60
1	D	203	ILE	N-CA-C	-6.28	94.05	111.00
1	A	10	ARG	CD-NE-CZ	6.07	132.10	123.60
1	C	203	ILE	N-CA-C	-5.99	94.83	111.00
1	A	203	ILE	N-CA-C	-5.59	95.92	111.00
1	B	203	ILE	N-CA-C	-5.54	96.03	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	2512	0	2537	48	0
1	B	2512	0	2537	45	0
1	C	2512	0	2537	56	0
1	D	2512	0	2537	54	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	36	0	20	1	0
3	B	36	0	20	2	0
3	C	44	0	26	3	0
3	D	44	0	26	2	0
4	A	61	0	0	3	0
4	B	68	0	0	2	0
4	C	50	0	0	1	0
4	D	49	0	0	3	0
All	All	10476	0	10240	191	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 9.

All (191) 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:80:GLU:HB2	1:A:110:LYS:HD3	1.32	1.05
1:B:120:ALA:HB2	3:B:336:SND:O3D	1.79	0.83
1:D:168:VAL:HG12	1:D:169:GLU:HG2	1.59	0.83
1:D:154:LEU:HD13	1:D:214:VAL:HG21	1.62	0.82
1:C:154:LEU:HD13	1:C:214:VAL:HG21	1.61	0.82
1:A:80:GLU:CB	1:A:110:LYS:HD3	2.12	0.80
1:B:154:LEU:HD13	1:B:214:VAL:HG21	1.64	0.80
1:A:154:LEU:HD13	1:A:214:VAL:HG21	1.67	0.76
1:C:168:VAL:HG12	1:C:169:GLU:HG2	1.67	0.75
1:C:80:GLU:HB2	1:C:110:LYS:HD3	1.68	0.74
1:C:149:CYS:HB3	3:C:337:SND:H4N	1.69	0.73
1:C:33:PRO:HG2	1:C:34:PHE:CD1	2.25	0.72
1:D:286:ASP:OD2	1:D:288:ARG:HD3	1.89	0.71
1:C:286:ASP:OD2	1:C:288:ARG:HD3	1.90	0.71
1:D:33:PRO:HG2	1:D:34:PHE:CD1	2.25	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:VAL:HG21	1:C:59:VAL:HG23	1.72	0.69
1:D:41:VAL:HG21	1:D:59:VAL:HG23	1.74	0.69
1:A:69:LYS:HB2	1:A:69:LYS:NZ	2.07	0.68
1:A:153:CYS:HA	1:A:290:SER:HB2	1.76	0.68
1:C:33:PRO:HG2	1:C:34:PHE:HD1	1.58	0.67
1:D:33:PRO:HG2	1:D:34:PHE:HD1	1.60	0.67
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.78	0.65
1:B:153:CYS:HA	1:B:290:SER:HB2	1.78	0.64
1:B:69:LYS:HB2	1:B:69:LYS:NZ	2.13	0.63
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.82	0.62
1:C:115:LYS:HE2	1:C:141:MET:O	2.00	0.62
1:D:171:LEU:HD23	1:D:226:THR:HG23	1.82	0.61
1:C:171:LEU:HD23	1:C:226:THR:HG23	1.83	0.61
1:A:286:ASP:OD2	1:A:288:ARG:HD3	2.00	0.61
1:A:114:LYS:O	1:A:115:LYS:HD2	2.00	0.60
1:D:115:LYS:HE2	1:D:141:MET:O	2.01	0.60
1:B:114:LYS:O	1:B:115:LYS:HD2	2.01	0.59
1:A:172:MET:HG2	1:A:173:THR:N	2.16	0.58
1:D:149:CYS:HB3	3:D:338:SND:H4N	1.86	0.58
1:B:286:ASP:OD2	1:B:288:ARG:HD3	2.03	0.58
1:C:83:PRO:CB	1:C:86:LYS:HG3	2.33	0.58
1:A:292:PHE:CE1	1:A:307:VAL:HG22	2.39	0.57
1:D:155:ALA:HB3	1:D:156:PRO:HD3	1.86	0.57
1:C:153:CYS:HA	1:C:290:SER:HB2	1.87	0.57
1:B:292:PHE:CE1	1:B:307:VAL:HG22	2.40	0.57
1:A:312:ASP:O	4:A:563:HOH:O	2.17	0.56
1:A:231:ARG:NH2	4:A:551:HOH:O	2.37	0.56
1:B:172:MET:HG2	1:B:173:THR:N	2.20	0.56
1:D:287:ASN:HB2	4:D:535:HOH:O	2.06	0.56
1:A:83:PRO:O	1:A:86:LYS:HB2	2.06	0.55
1:C:102:ILE:HG13	1:C:124:ASP:OD2	2.07	0.55
1:B:169:GLU:HB2	1:C:300:LEU:CD2	2.36	0.55
1:B:252:TYR:CE2	1:B:256:LYS:HD2	2.42	0.55
1:C:38:GLU:OE2	1:C:38:GLU:N	2.39	0.54
1:D:208:THR:HA	2:D:504:SO4:O2	2.08	0.54
1:D:330:LYS:O	1:D:334:ALA:HB2	2.08	0.53
1:C:83:PRO:HB3	1:C:86:LYS:HG3	1.89	0.53
1:A:286:ASP:OD1	1:A:288:ARG:NH1	2.41	0.53
1:B:286:ASP:OD1	1:B:288:ARG:NH1	2.42	0.53
1:D:153:CYS:HA	1:D:290:SER:HB2	1.91	0.53
1:A:252:TYR:CE2	1:A:256:LYS:HD2	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HD3	1:D:278:VAL:O	2.08	0.52
1:D:165:PHE:O	1:D:166:GLU:HB3	2.09	0.52
1:C:54:LYS:H	1:C:54:LYS:HD2	1.75	0.52
1:A:292:PHE:HE1	1:A:307:VAL:HG22	1.75	0.52
1:D:171:LEU:CD2	1:D:226:THR:HG23	2.40	0.52
1:D:109:PHE:CZ	1:D:142:LYS:HB3	2.44	0.52
1:B:231:ARG:NH2	4:B:573:HOH:O	2.42	0.52
1:C:165:PHE:O	1:C:166:GLU:HB3	2.10	0.52
1:D:54:LYS:H	1:D:54:LYS:HD2	1.74	0.52
1:A:236:ASN:O	1:A:237:VAL:HB	2.10	0.52
1:D:102:ILE:HG13	1:D:124:ASP:OD2	2.09	0.51
1:C:33:PRO:HB3	1:C:75:ASN:O	2.11	0.51
1:C:109:PHE:CZ	1:C:142:LYS:HB3	2.44	0.51
1:D:102:ILE:HD11	1:D:124:ASP:O	2.10	0.51
1:B:178:VAL:HG11	1:D:184:THR:HB	1.91	0.51
1:C:330:LYS:O	1:C:334:ALA:HB2	2.10	0.51
1:A:115:LYS:HE2	1:A:141:MET:O	2.11	0.51
1:B:188:PRO:HD3	4:D:538:HOH:O	2.09	0.51
1:D:172:MET:HG2	1:D:173:THR:N	2.24	0.51
1:B:194:ARG:NH2	1:C:295:LYS:HB2	2.25	0.51
1:A:41:VAL:HG21	1:A:59:VAL:HG23	1.93	0.51
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.92	0.50
1:A:243:THR:HG23	1:D:171:LEU:HD12	1.92	0.50
1:B:18:THR:HG21	1:B:319:GLN:HA	1.93	0.50
1:D:9:GLY:HA3	3:D:338:SND:O5B	2.11	0.50
1:A:18:THR:HG21	1:A:319:GLN:HA	1.92	0.50
1:A:178:VAL:HG11	1:C:184:THR:HB	1.94	0.50
1:D:38:GLU:N	1:D:38:GLU:OE2	2.42	0.50
1:A:69:LYS:HZ3	1:A:69:LYS:HB2	1.77	0.50
1:B:231:ARG:HH21	1:B:231:ARG:HG3	1.76	0.50
1:A:232:VAL:HG11	1:D:232:VAL:HG11	1.92	0.49
1:B:97:GLY:HA3	3:B:336:SND:H2D	1.93	0.49
1:B:41:VAL:HG21	1:B:59:VAL:HG23	1.94	0.49
1:D:236:ASN:O	1:D:237:VAL:HB	2.13	0.49
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.95	0.49
1:B:115:LYS:HE2	1:B:141:MET:O	2.13	0.49
1:C:171:LEU:CD2	1:C:226:THR:HG23	2.42	0.49
1:B:292:PHE:HE1	1:B:307:VAL:HG22	1.77	0.49
1:C:41:VAL:CG2	1:C:59:VAL:HG23	2.42	0.48
1:C:109:PHE:HZ	1:C:142:LYS:HB3	1.77	0.48
1:A:69:LYS:HZ2	1:A:69:LYS:HB2	1.79	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASN:O	1:B:237:VAL:HB	2.13	0.48
1:C:83:PRO:HB2	1:C:86:LYS:HG3	1.94	0.48
1:C:133:ASN:HA	1:C:135:GLU:OE1	2.14	0.48
1:B:69:LYS:HZ3	1:B:69:LYS:HB2	1.79	0.48
1:C:18:THR:HG21	1:C:319:GLN:HA	1.94	0.48
1:C:37:LEU:HD21	1:C:59:VAL:HG13	1.94	0.48
1:A:300:LEU:HD23	1:A:304:PHE:HD2	1.79	0.48
1:D:41:VAL:CG2	1:D:59:VAL:HG23	2.42	0.48
1:C:172:MET:HG2	1:C:173:THR:N	2.28	0.47
1:B:172:MET:CE	1:B:208:THR:HG21	2.45	0.47
1:D:109:PHE:HZ	1:D:142:LYS:HB3	1.78	0.47
1:B:52:MET:HE2	1:B:52:MET:HB3	1.69	0.47
1:C:102:ILE:HD11	1:C:124:ASP:O	2.14	0.47
1:C:31:ASN:ND2	3:C:337:SND:H2A	2.30	0.47
1:B:298:ILE:HG13	1:B:306:LYS:HB3	1.96	0.47
1:D:176:HIS:HB3	1:D:231:ARG:HD3	1.97	0.47
1:C:31:ASN:HD22	3:C:337:SND:H2A	1.80	0.47
1:C:260:LYS:O	1:C:264:GLU:HG3	2.14	0.47
1:D:18:THR:HG21	1:D:319:GLN:HA	1.96	0.46
1:A:298:ILE:HG13	1:A:306:LYS:HB3	1.97	0.46
1:B:69:LYS:HG2	4:B:548:HOH:O	2.16	0.46
1:B:194:ARG:HG2	1:C:277:ASP:HB3	1.97	0.46
1:B:300:LEU:HD23	1:B:304:PHE:HD2	1.81	0.46
1:D:106:SER:HA	1:D:109:PHE:CD2	2.50	0.46
1:A:325:ILE:O	1:A:329:GLN:HG3	2.15	0.46
1:D:33:PRO:HB3	1:D:75:ASN:O	2.16	0.46
1:A:231:ARG:HH21	1:A:231:ARG:HG3	1.79	0.46
1:A:242:LEU:HG	1:A:244:VAL:HG13	1.98	0.45
1:B:325:ILE:O	1:B:329:GLN:HG3	2.17	0.45
1:D:37:LEU:HD21	1:D:59:VAL:HG13	1.97	0.45
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.51	0.45
1:A:204:ILE:HB	1:A:231:ARG:HB2	1.98	0.45
1:B:252:TYR:CD2	1:B:256:LYS:HD2	2.51	0.45
1:C:106:SER:HA	1:C:109:PHE:CD2	2.52	0.45
1:B:238:SER:HB2	1:B:311:TYR:CZ	2.52	0.45
1:C:271:LEU:HD12	1:C:290:SER:O	2.16	0.45
1:A:120:ALA:HB2	3:A:335:SND:O3D	2.17	0.45
1:D:80:GLU:HB2	1:D:110:LYS:HG3	1.98	0.44
4:A:550:HOH:O	1:D:245:ARG:HG3	2.16	0.44
1:A:172:MET:CE	1:A:208:THR:HG21	2.47	0.44
1:B:194:ARG:HH21	1:C:295:LYS:HB2	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLU:C	1:C:23:GLY:H	2.21	0.44
1:A:169:GLU:HB2	1:D:300:LEU:CD2	2.48	0.44
1:C:236:ASN:O	1:C:237:VAL:HB	2.17	0.44
1:B:129:VAL:HG11	1:B:155:ALA:HB3	2.00	0.44
1:A:80:GLU:HB2	1:A:110:LYS:CD	2.24	0.44
1:B:169:GLU:HB2	1:C:300:LEU:HD21	1.98	0.44
1:D:9:GLY:O	1:D:13:ARG:HB2	2.17	0.44
1:A:252:TYR:CD2	1:A:256:LYS:HD2	2.53	0.44
1:A:117:ILE:N	1:A:117:ILE:HD12	2.33	0.43
1:B:11:ILE:O	1:B:15:VAL:HG23	2.19	0.43
1:D:30:VAL:HG12	1:D:31:ASN:N	2.34	0.43
1:D:13:ARG:NH1	4:D:538:HOH:O	2.51	0.43
1:B:204:ILE:HB	1:B:231:ARG:HB2	1.99	0.43
1:C:34:PHE:N	1:C:34:PHE:CD1	2.86	0.43
1:A:83:PRO:HB3	1:A:86:LYS:HG3	2.00	0.43
1:C:286:ASP:OD1	1:C:288:ARG:NH1	2.51	0.43
1:C:65:VAL:HA	1:C:69:LYS:O	2.19	0.43
1:D:65:VAL:HA	1:D:69:LYS:O	2.19	0.43
1:D:228:MET:HB2	1:D:228:MET:HE3	1.94	0.42
1:B:231:ARG:HG3	1:B:231:ARG:NH2	2.33	0.42
1:B:242:LEU:HG	1:B:244:VAL:HG13	2.01	0.42
1:D:21:GLU:C	1:D:23:GLY:H	2.22	0.42
1:B:41:VAL:HG13	1:B:57:VAL:HG12	2.00	0.42
1:D:260:LYS:O	1:D:264:GLU:HG3	2.19	0.42
1:D:34:PHE:N	1:D:34:PHE:CD1	2.87	0.42
1:A:129:VAL:HG11	1:A:155:ALA:HB3	2.01	0.42
1:A:8:PHE:CE2	1:A:13:ARG:HG2	2.55	0.42
1:A:8:PHE:CZ	1:A:13:ARG:HG2	2.55	0.42
1:C:298:ILE:O	1:C:305:VAL:HG23	2.20	0.42
1:C:78:LYS:HA	1:C:79:PRO:HD3	1.91	0.42
1:B:300:LEU:HD13	1:C:226:THR:HG22	2.02	0.42
1:A:76:GLU:HB2	1:A:82:ILE:HG12	2.01	0.42
1:B:260:LYS:O	1:B:264:GLU:HG3	2.19	0.42
1:C:30:VAL:HG12	1:C:31:ASN:N	2.35	0.42
1:D:286:ASP:OD1	1:D:288:ARG:NH1	2.53	0.42
1:D:60:GLU:O	1:D:61:ASP:HB2	2.20	0.42
1:C:325:ILE:O	1:C:329:GLN:HG3	2.20	0.42
1:A:231:ARG:HG3	1:A:231:ARG:NH2	2.36	0.41
1:A:260:LYS:O	1:A:264:GLU:HG3	2.21	0.41
1:B:110:LYS:HB3	1:B:110:LYS:HE3	1.87	0.41
1:D:76:GLU:OE2	1:D:76:GLU:HA	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HD2	4:C:525:HOH:O	2.21	0.41
1:D:298:ILE:O	1:D:305:VAL:HG23	2.21	0.41
1:D:325:ILE:O	1:D:329:GLN:HG3	2.21	0.41
1:D:171:LEU:HD23	1:D:226:THR:CG2	2.49	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.87	0.41
1:D:16:LEU:HD13	1:D:44:PHE:CE1	2.56	0.41
1:C:9:GLY:O	1:C:13:ARG:HB2	2.21	0.41
1:C:83:PRO:HB3	1:C:86:LYS:CG	2.51	0.40
1:D:79:PRO:HB2	1:D:107:ALA:CB	2.51	0.40
1:B:117:ILE:HD12	1:B:117:ILE:N	2.35	0.40
1:A:90:GLU:OE2	1:A:114:LYS:HE2	2.22	0.40
1:C:127:MET:HG2	1:C:145:SER:HB3	2.03	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	331/333 (99%)	313 (95%)	15 (4%)	3 (1%)	21	55
1	B	331/333 (99%)	313 (95%)	15 (4%)	3 (1%)	21	55
1	C	331/333 (99%)	304 (92%)	25 (8%)	2 (1%)	30	65
1	D	331/333 (99%)	305 (92%)	24 (7%)	2 (1%)	30	65
All	All	1324/1332 (99%)	1235 (93%)	79 (6%)	10 (1%)	24	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	B	313	ASN
1	A	237	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	237	VAL
1	C	237	VAL
1	D	237	VAL
1	A	166	GLU
1	B	166	GLU
1	C	166	GLU
1	D	166	GLU

### 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	272/272 (100%)	264 (97%)	8 (3%)	50	83
1	B	272/272 (100%)	264 (97%)	8 (3%)	50	83
1	C	272/272 (100%)	266 (98%)	6 (2%)	60	89
1	D	272/272 (100%)	267 (98%)	5 (2%)	66	91
All	All	1088/1088 (100%)	1061 (98%)	27 (2%)	55	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	16	LEU
1	A	69	LYS
1	A	115	LYS
1	A	154	LEU
1	A	307	VAL
1	A	314	GLU
1	A	319	GLN
1	B	1	SER
1	B	16	LEU
1	B	69	LYS
1	B	115	LYS
1	B	154	LEU
1	B	307	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	314	GLU
1	B	319	GLN
1	C	16	LEU
1	C	54	LYS
1	C	135	GLU
1	C	154	LEU
1	C	228	MET
1	C	319	GLN
1	D	16	LEU
1	D	54	LYS
1	D	154	LEU
1	D	228	MET
1	D	319	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	81	ASN
1	A	146	ASN
1	A	268	GLN
1	A	313	ASN
1	B	50	HIS
1	B	146	ASN
1	B	201	GLN
1	B	268	GLN
1	C	146	ASN
1	C	268	GLN
1	D	146	ASN
1	D	268	GLN

### 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 ⓘ

12 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	SND	A	335	-	32,39,48	0.98	2 (6%)	37,60,73	1.18	4 (10%)
2	SO4	A	501	-	4,4,4	3.10	3 (75%)	6,6,6	0.57	0
2	SO4	A	505	-	4,4,4	3.63	3 (75%)	6,6,6	0.42	0
3	SND	B	336	-	32,39,48	1.01	2 (6%)	37,60,73	1.18	3 (8%)
2	SO4	B	502	-	4,4,4	3.26	3 (75%)	6,6,6	0.55	0
2	SO4	B	506	-	4,4,4	3.97	4 (100%)	6,6,6	0.31	0
3	SND	C	337	-	38,48,48	5.16	8 (21%)	46,73,73	1.84	4 (8%)
2	SO4	C	503	-	4,4,4	3.52	3 (75%)	6,6,6	0.49	0
2	SO4	C	507	-	4,4,4	3.74	4 (100%)	6,6,6	0.51	0
3	SND	D	338	-	38,48,48	5.27	8 (21%)	46,73,73	1.84	4 (8%)
2	SO4	D	504	-	4,4,4	3.45	3 (75%)	6,6,6	0.34	0
2	SO4	D	508	-	4,4,4	3.86	3 (75%)	6,6,6	0.49	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	SND	A	335	-	-	0/18/54/62	0/4/4/5
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	505	-	-	0/0/0/0	0/0/0/0
3	SND	B	336	-	-	0/18/54/62	0/4/4/5
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	506	-	-	0/0/0/0	0/0/0/0
3	SND	C	337	-	-	0/22/62/62	0/5/5/5
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
3	SND	D	338	-	-	0/22/62/62	0/5/5/5
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	D	508	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	338	SND	C7N-S7N	-30.66	1.23	1.67
3	C	337	SND	C7N-S7N	-30.25	1.24	1.67
3	C	337	SND	C5A-N7A	-2.38	1.31	1.39
3	A	335	SND	PN-O2N	-2.21	1.45	1.54
3	D	338	SND	C5A-N7A	-2.13	1.32	1.39
3	D	338	SND	C2A-N3A	2.12	1.35	1.32
3	B	336	SND	C4A-N3A	2.18	1.38	1.35
2	C	507	SO4	O1-S	2.19	1.54	1.47
3	C	337	SND	C6N-N1N	2.41	1.41	1.35
3	D	338	SND	O4B-C1B	2.53	1.44	1.41
3	C	337	SND	C2A-N3A	2.59	1.36	1.32
3	D	338	SND	C6N-N1N	2.59	1.42	1.35
2	B	506	SO4	O1-S	2.59	1.56	1.47
3	C	337	SND	C7N-N7N	2.67	1.34	1.32
3	A	335	SND	C2A-N1A	2.70	1.39	1.33
3	B	336	SND	C2A-N1A	2.83	1.39	1.33
3	C	337	SND	O4B-C1B	3.06	1.45	1.41
3	D	338	SND	C7N-N7N	3.23	1.35	1.32
2	A	501	SO4	O2-S	3.24	1.58	1.47
2	C	503	SO4	O2-S	3.27	1.58	1.47
2	B	502	SO4	O2-S	3.29	1.58	1.47
2	A	501	SO4	O3-S	3.30	1.59	1.47
2	D	504	SO4	O2-S	3.58	1.59	1.47
2	B	506	SO4	O2-S	3.72	1.59	1.47
2	B	502	SO4	O3-S	3.73	1.60	1.47
2	D	508	SO4	O2-S	3.74	1.59	1.47
2	A	501	SO4	O4-S	3.79	1.61	1.47
2	A	505	SO4	O2-S	3.82	1.60	1.47
2	C	507	SO4	O2-S	3.86	1.60	1.47
3	C	337	SND	O4D-C1D	3.87	1.46	1.41
2	A	505	SO4	O3-S	3.93	1.61	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SO4	O4-S	3.95	1.61	1.47
2	D	504	SO4	O4-S	3.98	1.61	1.47
2	D	504	SO4	O3-S	4.04	1.61	1.47
2	D	508	SO4	O3-S	4.19	1.62	1.47
2	C	507	SO4	O3-S	4.22	1.62	1.47
2	C	507	SO4	O4-S	4.28	1.62	1.47
2	C	503	SO4	O4-S	4.32	1.62	1.47
2	C	503	SO4	O3-S	4.34	1.63	1.47
2	A	505	SO4	O4-S	4.35	1.63	1.47
2	B	506	SO4	O3-S	4.42	1.63	1.47
3	D	338	SND	O4D-C1D	4.45	1.46	1.41
3	C	337	SND	C3N-C7N	4.72	1.55	1.49
2	B	506	SO4	O4-S	4.79	1.64	1.47
2	D	508	SO4	O4-S	4.92	1.65	1.47
3	D	338	SND	C3N-C7N	5.73	1.56	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	338	SND	N3A-C2A-N1A	-9.71	121.46	128.89
3	C	337	SND	N3A-C2A-N1A	-9.34	121.74	128.89
3	A	335	SND	C1B-N9A-C4A	-3.69	121.37	126.94
3	B	336	SND	C1B-N9A-C4A	-3.65	121.43	126.94
3	D	338	SND	C4B-O4B-C1B	-3.53	105.84	109.72
3	C	337	SND	C4B-O4B-C1B	-3.50	105.87	109.72
3	C	337	SND	C4N-C3N-C7N	-2.94	118.40	120.95
3	D	338	SND	C4N-C3N-C7N	-2.03	119.19	120.95
3	A	335	SND	N3A-C2A-N1A	-2.01	127.36	128.89
3	B	336	SND	C1D-C2D-C3D	2.26	105.94	101.40
3	A	335	SND	O4D-C4D-C3D	2.29	109.75	105.15
3	A	335	SND	O3-PN-O5D	2.49	109.55	102.94
3	B	336	SND	O4D-C4D-C3D	2.52	110.22	105.15
3	D	338	SND	C4A-C5A-N7A	4.15	113.30	109.48
3	C	337	SND	C4A-C5A-N7A	4.30	113.44	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	335	SND	1	0
3	B	336	SND	2	0
3	C	337	SND	3	0
3	D	338	SND	2	0
2	D	504	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 ⓘ

### 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	333/333 (100%)	-0.56	3 (0%) 85 79	12, 26, 45, 69	0
1	B	333/333 (100%)	-0.61	4 (1%) 81 73	13, 24, 42, 67	0
1	C	333/333 (100%)	-0.27	13 (3%) 43 31	16, 31, 67, 84	0
1	D	333/333 (100%)	-0.28	5 (1%) 76 68	13, 31, 64, 82	0
All	All	1332/1332 (100%)	-0.43	25 (1%) 70 59	12, 27, 60, 84	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	334	ALA	10.3
1	C	334	ALA	6.9
1	A	334	ALA	6.2
1	B	334	ALA	5.9
1	C	81	ASN	4.5
1	D	333	SER	3.9
1	C	77	MET	3.5
1	C	61	ASP	3.1
1	C	78	LYS	3.0
1	C	80	GLU	3.0
1	A	333	SER	2.8
1	D	61	ASP	2.7
1	B	333	SER	2.6
1	B	191	LYS	2.6
1	C	52	MET	2.6
1	C	191	LYS	2.6
1	A	34	PHE	2.5
1	C	86	LYS	2.5
1	C	34	PHE	2.3
1	D	85	SER	2.2
1	B	21	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	22	MET	2.1
1	C	54	LYS	2.1
1	D	80	GLU	2.0
1	C	333	SER	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(Å <sup>2</sup> )	Q<0.9
2	SO4	D	504	5/5	0.94	0.33	9.84	22,22,24,39	0
2	SO4	C	503	5/5	0.95	0.27	4.46	22,22,24,40	0
2	SO4	A	501	5/5	0.96	0.23	3.25	22,22,23,38	0
3	SND	B	336	36/44	0.94	0.18	0.94	29,37,79,80	0
2	SO4	B	502	5/5	0.96	0.20	0.92	21,21,23,37	0
3	SND	A	335	36/44	0.94	0.18	0.18	36,41,90,91	0
3	SND	C	337	44/44	0.89	0.23	0.18	54,63,87,92	0
3	SND	D	338	44/44	0.95	0.17	-0.16	44,51,69,76	0
2	SO4	B	506	5/5	0.91	0.54	-	22,23,25,47	0
2	SO4	A	505	5/5	0.93	0.47	-	23,23,25,44	0
2	SO4	D	508	5/5	0.92	0.42	-	23,23,24,44	0
2	SO4	C	507	5/5	0.91	0.52	-	24,24,26,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.