



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:38 AM EDT

PDB ID : 7S77  
Title : Crystal structure of the G391V variant of human PGM-1  
Authors : Stiers, K.M.; Beamer, L.J.  
Deposited on : 2021-09-15  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

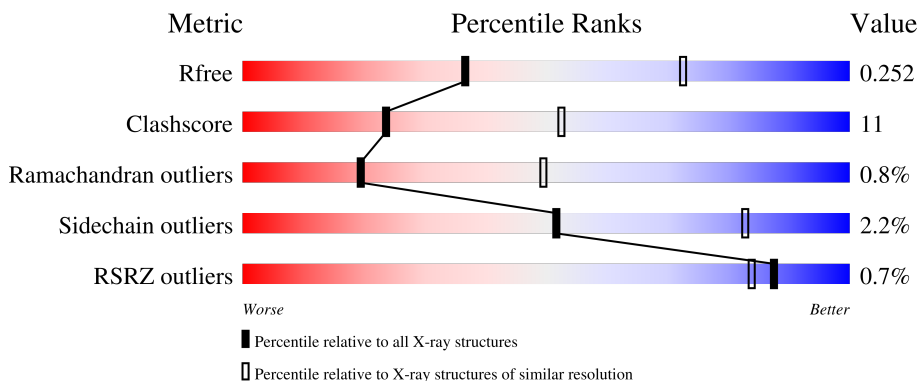
# 1 Overall quality at a glance

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 of 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	585	 0.252
1	B	585	 0.252

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7916 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 Phosphoglucomutase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4060	2583	693	767	17	0	1	0
1	B	529	3820	2426	654	727	13	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

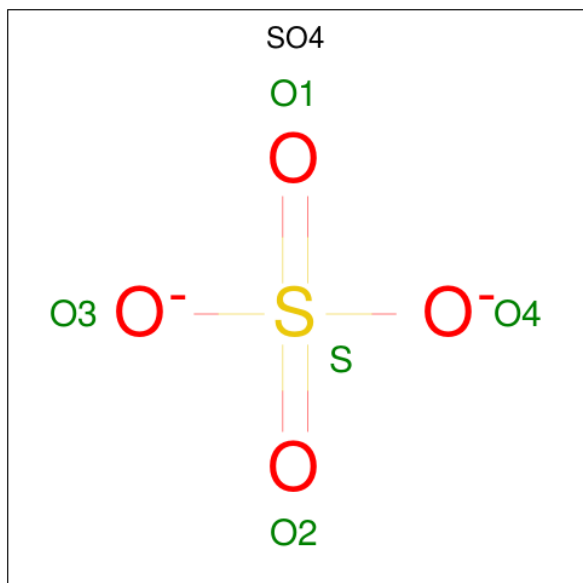
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P36871
A	-21	HIS	-	expression tag	UNP P36871
A	-20	HIS	-	expression tag	UNP P36871
A	-19	HIS	-	expression tag	UNP P36871
A	-18	HIS	-	expression tag	UNP P36871
A	-17	HIS	-	expression tag	UNP P36871
A	-16	HIS	-	expression tag	UNP P36871
A	-15	SER	-	expression tag	UNP P36871
A	-14	SER	-	expression tag	UNP P36871
A	-13	GLY	-	expression tag	UNP P36871
A	-12	VAL	-	expression tag	UNP P36871
A	-11	ASP	-	expression tag	UNP P36871
A	-10	LEU	-	expression tag	UNP P36871
A	-9	GLY	-	expression tag	UNP P36871
A	-8	THR	-	expression tag	UNP P36871
A	-7	GLU	-	expression tag	UNP P36871
A	-6	ASN	-	expression tag	UNP P36871
A	-5	LEU	-	expression tag	UNP P36871
A	-4	TYR	-	expression tag	UNP P36871
A	-3	PHE	-	expression tag	UNP P36871
A	-2	GLN	-	expression tag	UNP P36871
A	-1	SER	-	expression tag	UNP P36871
A	0	ASN	-	expression tag	UNP P36871
A	391	VAL	GLY	engineered mutation	UNP P36871
B	-22	MET	-	initiating methionine	UNP P36871

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P36871
B	-20	HIS	-	expression tag	UNP P36871
B	-19	HIS	-	expression tag	UNP P36871
B	-18	HIS	-	expression tag	UNP P36871
B	-17	HIS	-	expression tag	UNP P36871
B	-16	HIS	-	expression tag	UNP P36871
B	-15	SER	-	expression tag	UNP P36871
B	-14	SER	-	expression tag	UNP P36871
B	-13	GLY	-	expression tag	UNP P36871
B	-12	VAL	-	expression tag	UNP P36871
B	-11	ASP	-	expression tag	UNP P36871
B	-10	LEU	-	expression tag	UNP P36871
B	-9	GLY	-	expression tag	UNP P36871
B	-8	THR	-	expression tag	UNP P36871
B	-7	GLU	-	expression tag	UNP P36871
B	-6	ASN	-	expression tag	UNP P36871
B	-5	LEU	-	expression tag	UNP P36871
B	-4	TYR	-	expression tag	UNP P36871
B	-3	PHE	-	expression tag	UNP P36871
B	-2	GLN	-	expression tag	UNP P36871
B	-1	SER	-	expression tag	UNP P36871
B	0	ASN	-	expression tag	UNP P36871
B	391	VAL	GLY	engineered mutation	UNP P36871

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



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

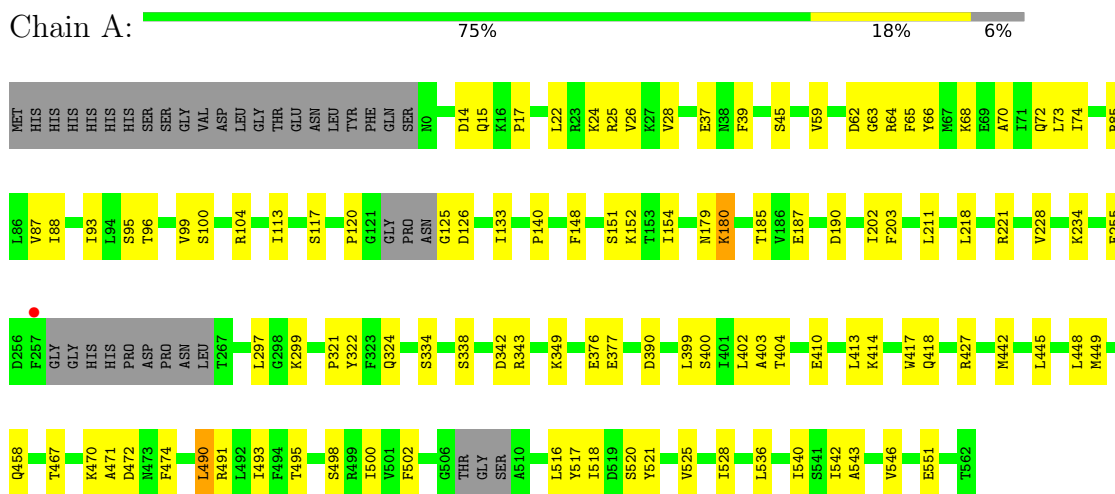
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	14	Total	O	0	0
			14	14		

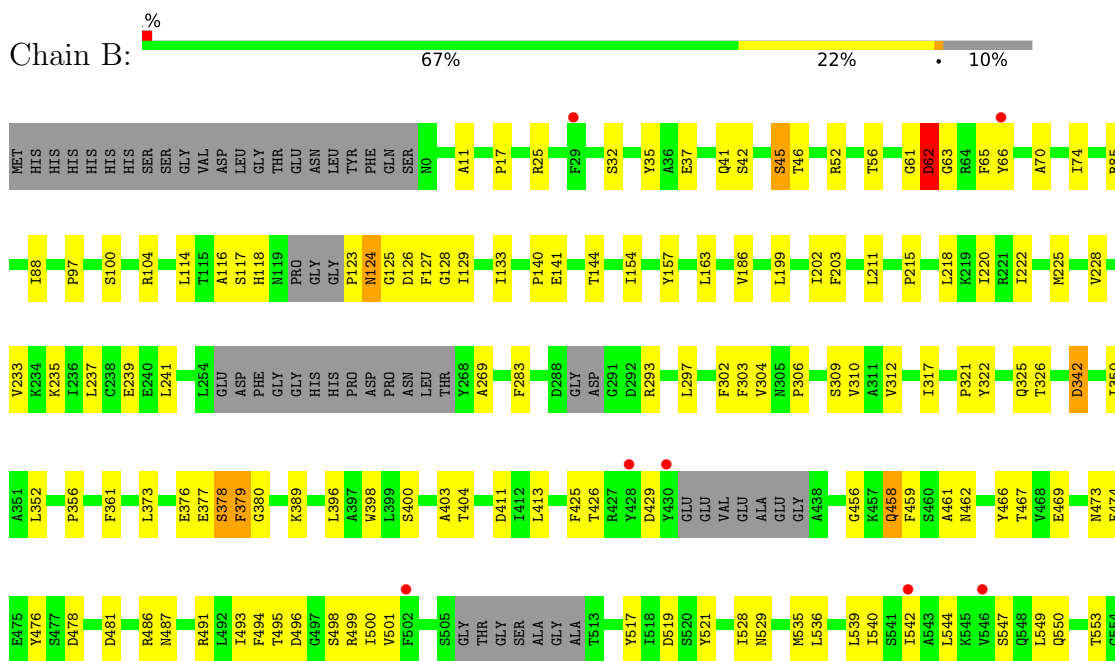
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoglucumutase-1



- Molecule 1: Phosphoglucumutase-1



R556
THR
ALA
P558
T559
V560
I561
I562

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.05Å 171.05Å 100.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.80 48.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.18-2.80) 99.9 (48.18-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.193 , 0.252 0.193 , 0.252	Depositor DCC
$R_{free}$ test set	1862 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.7	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.49	0/4134	0.66	1/5609 (0.0%)
1	B	0.46	1/3891 (0.0%)	0.66	1/5297 (0.0%)
All	All	0.47	1/8025 (0.0%)	0.66	2/10906 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TYR	CE1-CZ	-6.41	1.30	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	62	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4060	0	3942	75	0
1	B	3820	0	3529	99	0
2	A	5	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	0	2	1
3	B	14	0	0	3	0
All	All	7916	0	7471	172	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 11.

All (172) 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:442:MET:HE2	1:A:490:LEU:CD1	1.46	1.42
1:A:442:MET:CE	1:A:490:LEU:CD1	2.07	1.33
1:A:442:MET:CE	1:A:490:LEU:HD12	1.60	1.29
1:A:442:MET:HE1	1:A:490:LEU:HD12	1.29	1.12
1:A:442:MET:HE2	1:A:490:LEU:HD11	1.30	1.08
1:A:518:ILE:HD13	1:A:540:ILE:HD13	1.39	1.02
1:B:486:ARG:HH11	1:B:486:ARG:HB2	1.28	0.98
1:B:486:ARG:HB2	1:B:486:ARG:NH1	1.81	0.95
1:A:449:MET:HE1	1:A:490:LEU:HD22	1.53	0.89
1:B:123:PRO:O	1:B:125:GLY:N	2.13	0.80
1:A:442:MET:CE	1:A:490:LEU:HD13	2.11	0.80
1:B:429:ASP:HB2	1:B:560:VAL:HG23	1.63	0.80
1:A:518:ILE:CD1	1:A:540:ILE:HD13	2.13	0.79
1:A:45:SER:OG	3:A:701:HOH:O	2.02	0.76
1:A:190:ASP:O	3:A:702:HOH:O	2.03	0.75
1:B:211:LEU:HD11	1:B:218:LEU:HD13	1.70	0.74
1:B:302:PHE:HE2	1:B:413:LEU:HD13	1.54	0.72
1:B:62:ASP:O	1:B:228:VAL:HG22	1.89	0.72
1:B:56:THR:HG21	1:B:85:ARG:HE	1.54	0.71
1:B:486:ARG:HH11	1:B:486:ARG:CB	2.02	0.71
1:B:62:ASP:HA	1:B:228:VAL:CG2	2.22	0.70
1:B:41:GLN:HG3	1:B:157:TYR:HB2	1.71	0.70
1:B:376:GLU:HG2	1:B:378:SER:HB3	1.75	0.68
1:B:528:ILE:HD12	1:B:529:ASN:HB2	1.76	0.67
1:B:62:ASP:HA	1:B:228:VAL:HG21	1.74	0.67
1:B:549:LEU:O	1:B:553:THR:HG22	1.94	0.67
1:B:429:ASP:HB2	1:B:560:VAL:CG2	2.25	0.67
1:B:141:GLU:HA	1:B:144:THR:HG22	1.76	0.66
1:B:494:PHE:HE2	1:B:500:ILE:HG13	1.62	0.65
1:B:70:ALA:O	1:B:74:ILE:HD12	1.97	0.65
1:A:37:GLU:HG3	1:A:73:LEU:HD11	1.79	0.63

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:SER:HB2	1:B:398:TRP:HE1	1.63	0.63
1:B:499:ARG:NH1	1:B:519:ASP:OD2	2.30	0.63
1:A:472:ASP:OD1	1:A:491:ARG:HD3	1.99	0.62
1:A:179:ASN:C	1:A:180:LYS:HD2	2.19	0.62
1:B:473:ASN:HD21	1:B:487:ASN:HA	1.63	0.61
1:B:469:GLU:OE2	1:B:495:THR:HA	2.00	0.61
1:B:535:MET:SD	1:B:535:MET:N	2.73	0.61
1:B:540:ILE:O	1:B:544:LEU:HD22	2.01	0.60
1:A:26:VAL:HG12	1:A:125:GLY:O	2.02	0.60
1:B:199:LEU:HD13	1:B:396:LEU:HD22	1.84	0.59
1:B:493:ILE:HG13	1:B:499:ARG:HG2	1.85	0.59
1:B:474:PHE:HB2	1:B:491:ARG:HD2	1.84	0.58
1:B:100:SER:O	1:B:104:ARG:HG3	2.04	0.58
1:B:356:PRO:HD3	1:B:476:TYR:CG	2.39	0.58
1:B:45:SER:HA	1:B:52:ARG:NH2	2.19	0.58
1:A:349:LYS:NZ	1:B:203:PHE:O	2.37	0.56
1:B:61:GLY:O	1:B:63:GLY:N	2.39	0.56
1:A:449:MET:CE	1:A:490:LEU:HD22	2.33	0.56
1:A:525:VAL:HA	1:A:528:ILE:HG12	1.87	0.55
1:B:400:SER:O	1:B:404:THR:HG23	2.06	0.55
1:B:220:ILE:HD12	1:B:222:ILE:HD13	1.88	0.55
1:A:148:PHE:CZ	1:A:152:LYS:HD2	2.42	0.55
1:A:87:VAL:HG22	1:A:187:GLU:HB2	1.88	0.54
1:A:470:LYS:HD2	1:A:493:ILE:HD13	1.88	0.54
1:A:62:ASP:O	1:A:228:VAL:HG22	2.06	0.54
1:B:123:PRO:C	1:B:125:GLY:H	2.09	0.54
1:B:225:MET:CE	1:B:269:ALA:HA	2.38	0.54
1:B:306:PRO:O	1:B:310:VAL:HG23	2.08	0.54
1:A:536:LEU:O	1:A:540:ILE:HG12	2.07	0.54
1:A:458:GLN:HG2	1:A:467:THR:HB	1.89	0.53
1:A:551:GLU:OE1	1:A:551:GLU:N	2.38	0.53
1:B:501:VAL:HG13	1:B:517:TYR:HB2	1.90	0.53
1:B:211:LEU:HD22	1:B:403:ALA:HB2	1.91	0.53
1:B:118:HIS:N	3:B:603:HOH:O	2.41	0.53
1:B:469:GLU:CD	1:B:495:THR:HA	2.29	0.53
1:A:63:GLY:HA2	1:A:93:ILE:HD11	1.89	0.52
1:B:220:ILE:HG22	1:B:283:PHE:HB3	1.89	0.52
1:A:413:LEU:HD12	1:A:417:TRP:CZ2	2.45	0.52
1:B:32:SER:HB2	1:B:35:TYR:HB2	1.91	0.52
1:B:459:PHE:HB3	1:B:542:ILE:HD13	1.92	0.52
1:B:128:GLY:O	1:B:129:ILE:HD13	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLY:O	1:B:458:GLN:OE1	2.28	0.52
1:B:237:LEU:HD23	1:B:241:LEU:HD12	1.92	0.52
1:B:496:ASP:OD1	1:B:498:SER:HB3	2.10	0.51
1:B:501:VAL:HG13	1:B:517:TYR:CD1	2.46	0.51
1:B:553:THR:HG23	1:B:555:ARG:H	1.74	0.51
1:A:542:ILE:O	1:A:546:VAL:HG23	2.11	0.51
1:B:235:LYS:HA	1:B:239:GLU:HG3	1.93	0.51
1:B:498:SER:HB2	1:B:521:TYR:H	1.75	0.51
1:A:180:LYS:HD2	1:A:180:LYS:N	2.25	0.51
1:B:45:SER:HA	1:B:52:ARG:HH22	1.75	0.51
1:B:62:ASP:C	1:B:228:VAL:HG22	2.32	0.50
1:B:293:ARG:O	1:B:293:ARG:HG3	2.11	0.50
1:B:317:ILE:HD13	1:B:373:LEU:HD22	1.94	0.50
1:A:221:ARG:HH11	1:A:221:ARG:HG3	1.76	0.50
1:A:14:ASP:O	1:A:24:LYS:NZ	2.44	0.50
1:A:95:SER:O	1:A:99:VAL:HG23	2.13	0.49
1:A:400:SER:O	1:A:404:THR:HG23	2.13	0.49
1:A:502:PHE:CE2	1:A:516:LEU:HD13	2.47	0.49
1:A:343:ARG:HD2	1:A:521:TYR:CE2	2.47	0.49
1:B:501:VAL:CG1	1:B:517:TYR:HB2	2.43	0.49
1:B:304:VAL:HG12	1:B:413:LEU:HD11	1.95	0.49
1:B:124:ASN:HA	3:B:613:HOH:O	2.13	0.48
1:A:410:GLU:HG2	1:A:414:LYS:HE3	1.95	0.48
1:B:342:ASP:HA	1:B:352:LEU:HD22	1.96	0.48
1:A:324:GLN:HG2	1:B:350:ILE:HD11	1.95	0.48
1:B:467:THR:H	1:B:495:THR:HG23	1.79	0.48
1:A:117:SER:HB3	1:A:126:ASP:OD1	2.14	0.47
1:B:42:SER:O	1:B:46:THR:HG23	2.14	0.47
1:A:70:ALA:O	1:A:74:ILE:HG13	2.15	0.47
1:A:502:PHE:CZ	1:A:516:LEU:HD13	2.49	0.47
1:A:96:THR:HG23	1:A:113:ILE:HD13	1.97	0.47
1:B:37:GLU:OE2	1:B:37:GLU:N	2.46	0.47
1:B:56:THR:HG22	1:B:85:ARG:HG2	1.97	0.47
1:B:141:GLU:CA	1:B:144:THR:HG22	2.44	0.47
1:B:88:ILE:HD12	1:B:186:VAL:HG13	1.97	0.46
1:A:202:ILE:HG23	1:A:322:TYR:HB2	1.96	0.46
1:B:297:LEU:HD23	1:B:303:PHE:HA	1.97	0.46
1:B:426:THR:HG22	1:B:536:LEU:HD13	1.97	0.46
1:B:462:ASN:N	1:B:462:ASN:HD22	2.12	0.46
1:A:498:SER:OG	1:A:520:SER:HA	2.16	0.46
1:B:25:ARG:HA	1:B:126:ASP:HA	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:GLU:OE1	1:B:425:PHE:HE2	1.99	0.46
1:B:133:ILE:HD13	1:B:140:PRO:HD3	1.97	0.46
1:B:461:ALA:HB2	1:B:542:ILE:HG13	1.98	0.46
1:B:114:LEU:HD22	1:B:129:ILE:HD12	1.98	0.45
1:B:97:PRO:HG3	1:B:389:LYS:O	2.17	0.45
1:A:449:MET:HE1	1:A:490:LEU:CD2	2.37	0.45
1:B:342:ASP:CG	1:B:352:LEU:HD21	2.37	0.44
1:B:478:ASP:HB3	1:B:481:ASP:OD1	2.17	0.44
1:B:379:PHE:CG	1:B:380:GLY:N	2.85	0.44
1:B:312:VAL:HG21	1:B:398:TRP:CH2	2.52	0.44
1:A:15:GLN:HG2	1:A:22:LEU:HD21	2.00	0.44
1:B:62:ASP:HA	1:B:228:VAL:HG22	1.97	0.44
1:B:65:PHE:HB2	3:B:611:HOH:O	2.17	0.44
1:B:141:GLU:HA	1:B:144:THR:CG2	2.44	0.44
1:B:312:VAL:HG21	1:B:398:TRP:CZ2	2.52	0.44
1:A:64:ARG:HA	1:A:255:GLU:HA	1.99	0.44
1:B:202:ILE:HA	1:B:322:TYR:HB2	1.98	0.44
1:A:25:ARG:O	1:A:28:VAL:HG12	2.18	0.44
1:B:117:SER:OG	1:B:118:HIS:N	2.51	0.44
1:A:334:SER:HB3	1:A:376:GLU:HG2	1.99	0.43
1:A:59:VAL:CG1	1:A:88:ILE:HG12	2.48	0.43
1:A:221:ARG:HG3	1:A:221:ARG:NH1	2.33	0.43
1:A:179:ASN:O	1:A:180:LYS:HD2	2.18	0.43
1:A:449:MET:HB2	1:A:449:MET:HE2	1.75	0.43
1:B:356:PRO:HD2	1:B:361:PHE:CD1	2.53	0.43
1:A:62:ASP:HA	1:A:228:VAL:CG2	2.49	0.43
1:A:474:PHE:HB2	1:A:491:ARG:HD2	2.00	0.43
1:B:11:ALA:HA	1:B:154:ILE:HD11	1.99	0.43
1:B:56:THR:CG2	1:B:85:ARG:HG2	2.49	0.43
1:B:321:PRO:O	1:B:325:GLN:HG3	2.18	0.43
1:A:151:SER:O	1:A:154:ILE:HG22	2.18	0.43
1:A:500:ILE:HD13	1:A:543:ALA:HB2	2.01	0.42
1:A:62:ASP:HA	1:A:228:VAL:HG21	2.01	0.42
1:A:377:GLU:OE2	1:A:427:ARG:NH1	2.50	0.42
1:B:322:TYR:O	1:B:326:THR:HG23	2.19	0.42
1:A:445:LEU:O	1:A:448:LEU:HB2	2.19	0.42
1:A:85:ARG:HA	1:A:185:THR:O	2.20	0.42
1:A:120:PRO:HA	1:A:125:GLY:HA3	2.00	0.42
1:B:220:ILE:HD12	1:B:222:ILE:CD1	2.49	0.41
1:A:22:LEU:HD22	1:A:39:PHE:CD1	2.55	0.41
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.81	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:CD	1:A:427:ARG:HH11	2.23	0.41
1:A:203:PHE:HA	1:A:321:PRO:HD2	2.03	0.41
1:A:517:TYR:C	1:A:518:ILE:HG13	2.41	0.41
1:B:486:ARG:NH1	1:B:486:ARG:CB	2.68	0.41
1:B:539:LEU:HA	1:B:539:LEU:HD23	1.61	0.41
1:B:459:PHE:CB	1:B:542:ILE:HD13	2.51	0.41
1:A:100:SER:O	1:A:104:ARG:HG3	2.21	0.41
1:A:133:ILE:HD13	1:A:140:PRO:HD3	2.02	0.41
1:A:399:LEU:HD23	1:A:402:LEU:HD12	2.03	0.41
1:A:467:THR:HG23	1:A:495:THR:HG23	2.02	0.41
1:B:222:ILE:HG21	1:B:233:VAL:HG21	2.02	0.41
1:A:211:LEU:HD13	1:A:403:ALA:HA	2.03	0.41
1:A:442:MET:HE1	1:A:490:LEU:CD1	2.04	0.40
1:A:65:PHE:O	1:A:66:TYR:HB2	2.20	0.40
1:A:68:LYS:O	1:A:72:GLN:HG2	2.21	0.40
1:A:442:MET:HE2	1:A:490:LEU:HD12	1.33	0.40
1:B:116:ALA:HB2	1:B:127:PHE:HD1	1.86	0.40
1:A:449:MET:HB3	1:A:471: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)
3:A:705:HOH:O	3:A:705:HOH:O[8_555]	1.94	0.26

## 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	541/585 (92%)	520 (96%)	20 (4%)	1 (0%)	47 78
1	B	516/585 (88%)	475 (92%)	34 (7%)	7 (1%)	11 34

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1057/1170 (90%)	995 (94%)	54 (5%)	8 (1%)	19	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	ASP
1	B	124	ASN
1	B	550	GLN
1	B	45	SER
1	B	215	PRO
1	A	17	PRO
1	B	17	PRO
1	B	379	PHE

### 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	410/484 (85%)	401 (98%)	9 (2%)	52	83
1	B	363/484 (75%)	355 (98%)	8 (2%)	52	83
All	All	773/968 (80%)	756 (98%)	17 (2%)	52	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	218	LEU
1	A	234	LYS
1	A	297	LEU
1	A	299	LYS
1	A	338	SER
1	A	342	ASP
1	A	418	GLN
1	A	490	LEU
1	B	66	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	163	LEU
1	B	342	ASP
1	B	378	SER
1	B	411	ASP
1	B	458	GLN
1	B	547	SER
1	B	555	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	462	ASN
1	B	462	ASN
1	B	473	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	0.17	0	6,6,6	0.19	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 [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	548/585 (93%)	-0.55	1 (0%) 95 94	42, 67, 109, 165	0
1	B	529/585 (90%)	-0.34	7 (1%) 77 72	48, 92, 151, 198	0
All	All	1077/1170 (92%)	-0.45	8 (0%) 87 84	42, 77, 140, 198	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	TYR	3.9
1	B	502	PHE	3.0
1	B	29	PHE	2.7
1	B	430	TYR	2.5
1	A	257	PHE	2.2
1	B	546	VAL	2.1
1	B	66	TYR	2.1
1	B	542	ILE	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 monosaccharides 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(Å <sup>2</sup> )	Q < 0.9
2	SO4	A	601	5/5	0.90	0.20	144,147,149,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.