



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:13 AM UTC

PDB ID : 6D23 / pdb_00006d23
Title : GLUCOSE-6-P DEHYDROGENASE (APO FORM) FROM TRY-
PANOSOMA CRUZI
Authors : Botti, H.; Ortiz, C.; Comini, M.A.; Larrieux, N.; Buschiazzo, A.
Deposited on : 2018-04-12
Resolution : 2.85 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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

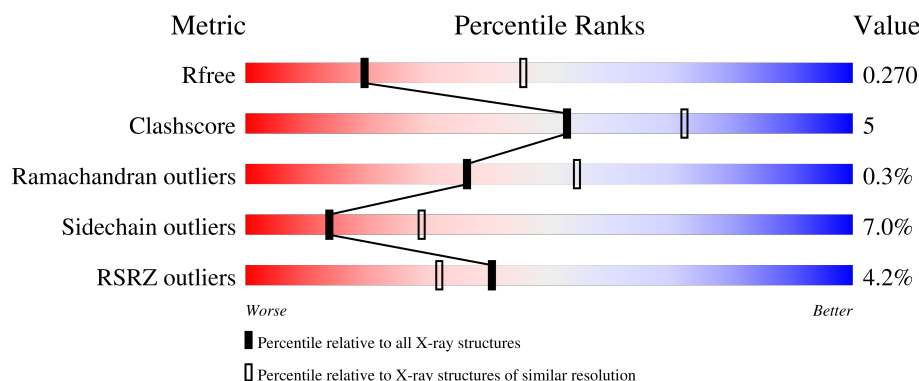
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 ≥ 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	541	4% 72% 16% • 10%
1	B	541	3% 74% 16% • 9%
1	C	541	4% 74% 16% • 9%
1	D	541	4% 74% 16% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15846 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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	3	0
			3858	2446	684	713	15			
1	B	490	Total	C	N	O	S	0	1	0
			3857	2445	675	722	15			
1	C	494	Total	C	N	O	S	0	3	0
			3900	2472	686	726	16			
1	D	494	Total	C	N	O	S	0	2	0
			3893	2468	684	725	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP Q1WBU6
A	16	GLY	-	expression tag	UNP Q1WBU6
A	17	SER	-	expression tag	UNP Q1WBU6
A	18	SER	-	expression tag	UNP Q1WBU6
A	19	HIS	-	expression tag	UNP Q1WBU6
A	20	HIS	-	expression tag	UNP Q1WBU6
A	21	HIS	-	expression tag	UNP Q1WBU6
A	22	HIS	-	expression tag	UNP Q1WBU6
A	23	HIS	-	expression tag	UNP Q1WBU6
A	24	HIS	-	expression tag	UNP Q1WBU6
A	25	SER	-	expression tag	UNP Q1WBU6
A	26	SER	-	expression tag	UNP Q1WBU6
A	27	GLY	-	expression tag	UNP Q1WBU6
A	28	LEU	-	expression tag	UNP Q1WBU6
A	29	VAL	-	expression tag	UNP Q1WBU6
A	30	PRO	-	expression tag	UNP Q1WBU6
A	31	ARG	-	expression tag	UNP Q1WBU6
A	32	GLY	-	expression tag	UNP Q1WBU6
A	33	SER	-	expression tag	UNP Q1WBU6
A	34	HIS	-	expression tag	UNP Q1WBU6
A	35	MET	-	expression tag	UNP Q1WBU6

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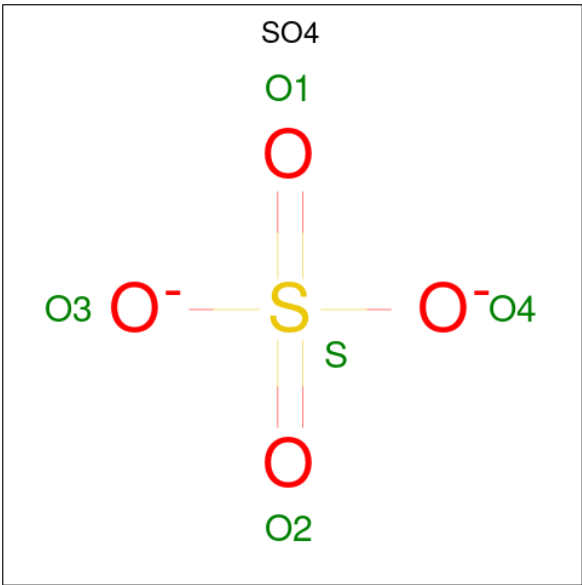
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	-	expression tag	UNP Q1WBU6
A	37	SER	-	expression tag	UNP Q1WBU6
A	290	GLU	ALA	conflict	UNP Q1WBU6
B	15	MET	-	expression tag	UNP Q1WBU6
B	16	GLY	-	expression tag	UNP Q1WBU6
B	17	SER	-	expression tag	UNP Q1WBU6
B	18	SER	-	expression tag	UNP Q1WBU6
B	19	HIS	-	expression tag	UNP Q1WBU6
B	20	HIS	-	expression tag	UNP Q1WBU6
B	21	HIS	-	expression tag	UNP Q1WBU6
B	22	HIS	-	expression tag	UNP Q1WBU6
B	23	HIS	-	expression tag	UNP Q1WBU6
B	24	HIS	-	expression tag	UNP Q1WBU6
B	25	SER	-	expression tag	UNP Q1WBU6
B	26	SER	-	expression tag	UNP Q1WBU6
B	27	GLY	-	expression tag	UNP Q1WBU6
B	28	LEU	-	expression tag	UNP Q1WBU6
B	29	VAL	-	expression tag	UNP Q1WBU6
B	30	PRO	-	expression tag	UNP Q1WBU6
B	31	ARG	-	expression tag	UNP Q1WBU6
B	32	GLY	-	expression tag	UNP Q1WBU6
B	33	SER	-	expression tag	UNP Q1WBU6
B	34	HIS	-	expression tag	UNP Q1WBU6
B	35	MET	-	expression tag	UNP Q1WBU6
B	36	ALA	-	expression tag	UNP Q1WBU6
B	37	SER	-	expression tag	UNP Q1WBU6
B	290	GLU	ALA	conflict	UNP Q1WBU6
C	15	MET	-	expression tag	UNP Q1WBU6
C	16	GLY	-	expression tag	UNP Q1WBU6
C	17	SER	-	expression tag	UNP Q1WBU6
C	18	SER	-	expression tag	UNP Q1WBU6
C	19	HIS	-	expression tag	UNP Q1WBU6
C	20	HIS	-	expression tag	UNP Q1WBU6
C	21	HIS	-	expression tag	UNP Q1WBU6
C	22	HIS	-	expression tag	UNP Q1WBU6
C	23	HIS	-	expression tag	UNP Q1WBU6
C	24	HIS	-	expression tag	UNP Q1WBU6
C	25	SER	-	expression tag	UNP Q1WBU6
C	26	SER	-	expression tag	UNP Q1WBU6
C	27	GLY	-	expression tag	UNP Q1WBU6
C	28	LEU	-	expression tag	UNP Q1WBU6
C	29	VAL	-	expression tag	UNP Q1WBU6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PRO	-	expression tag	UNP Q1WBU6
C	31	ARG	-	expression tag	UNP Q1WBU6
C	32	GLY	-	expression tag	UNP Q1WBU6
C	33	SER	-	expression tag	UNP Q1WBU6
C	34	HIS	-	expression tag	UNP Q1WBU6
C	35	MET	-	expression tag	UNP Q1WBU6
C	36	ALA	-	expression tag	UNP Q1WBU6
C	37	SER	-	expression tag	UNP Q1WBU6
C	290	GLU	ALA	conflict	UNP Q1WBU6
D	15	MET	-	expression tag	UNP Q1WBU6
D	16	GLY	-	expression tag	UNP Q1WBU6
D	17	SER	-	expression tag	UNP Q1WBU6
D	18	SER	-	expression tag	UNP Q1WBU6
D	19	HIS	-	expression tag	UNP Q1WBU6
D	20	HIS	-	expression tag	UNP Q1WBU6
D	21	HIS	-	expression tag	UNP Q1WBU6
D	22	HIS	-	expression tag	UNP Q1WBU6
D	23	HIS	-	expression tag	UNP Q1WBU6
D	24	HIS	-	expression tag	UNP Q1WBU6
D	25	SER	-	expression tag	UNP Q1WBU6
D	26	SER	-	expression tag	UNP Q1WBU6
D	27	GLY	-	expression tag	UNP Q1WBU6
D	28	LEU	-	expression tag	UNP Q1WBU6
D	29	VAL	-	expression tag	UNP Q1WBU6
D	30	PRO	-	expression tag	UNP Q1WBU6
D	31	ARG	-	expression tag	UNP Q1WBU6
D	32	GLY	-	expression tag	UNP Q1WBU6
D	33	SER	-	expression tag	UNP Q1WBU6
D	34	HIS	-	expression tag	UNP Q1WBU6
D	35	MET	-	expression tag	UNP Q1WBU6
D	36	ALA	-	expression tag	UNP Q1WBU6
D	37	SER	-	expression tag	UNP Q1WBU6
D	290	GLU	ALA	conflict	UNP Q1WBU6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



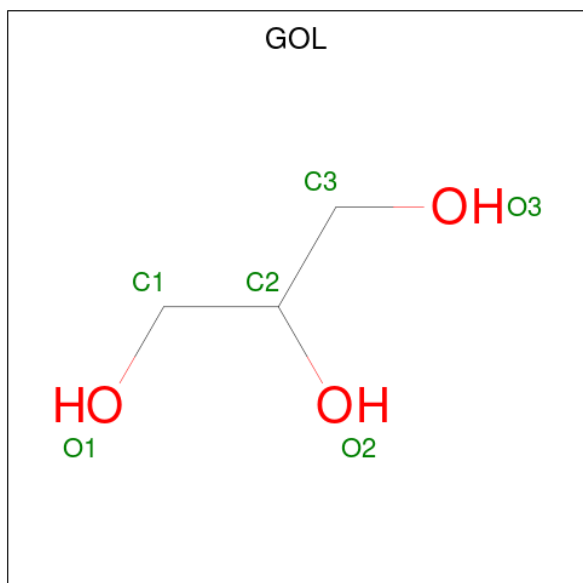
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O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

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

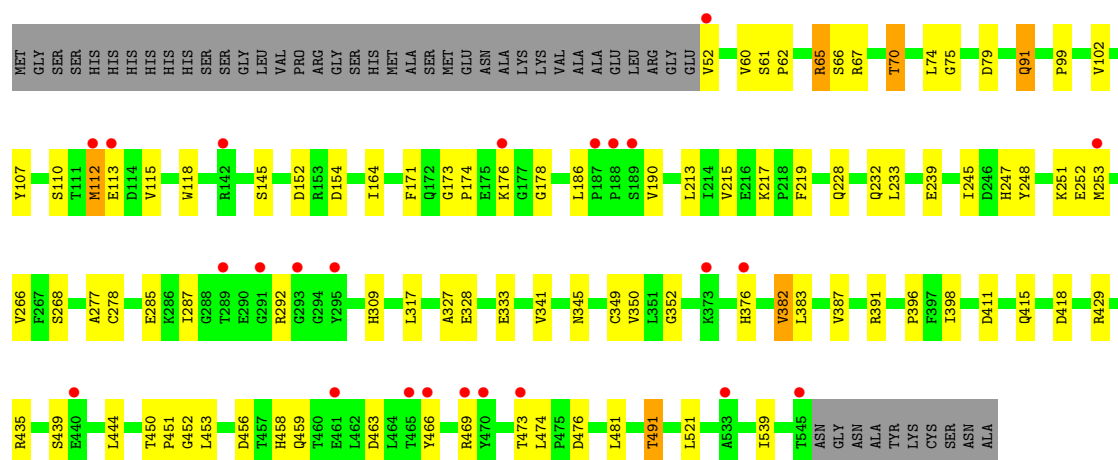
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Cl 5 5	0	0
4	B	4	Total Cl 4 4	0	0
4	C	9	Total Cl 9 9	0	0
4	D	5	Total Cl 5 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	8	Total O 8 8	0	0
5	C	22	Total O 22 22	0	0
5	D	29	Total O 29 29	0	0

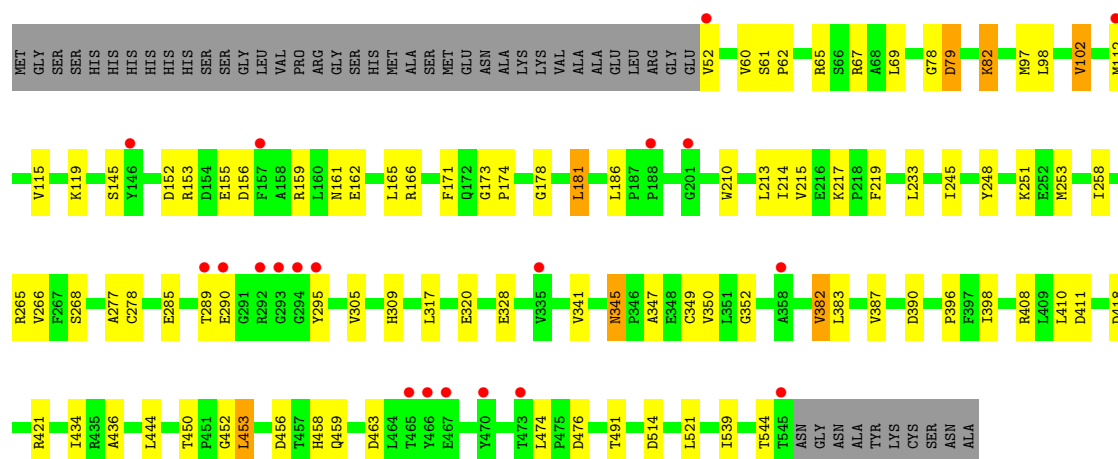
● Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain C:  4% 74% 16% 9%



● Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain D:  4% 74% 16% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.61Å 132.96Å 107.83Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	29.63 – 2.85 29.63 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.63-2.85) 98.9 (29.63-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.85Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.204 , 0.249 0.219 , 0.270	Depositor DCC
R_{free} test set	1257 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtrriage
Anisotropy	0.340	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6399e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, GOL

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	0.85	0/3945	1.36	19/5344 (0.4%)
1	B	0.87	1/3938 (0.0%)	1.39	20/5342 (0.4%)
1	C	0.89	1/3988 (0.0%)	1.37	19/5407 (0.4%)
1	D	0.88	0/3977	1.36	13/5393 (0.2%)
All	All	0.88	2/15848 (0.0%)	1.37	71/21486 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	MET	SD-CE	-5.67	1.65	1.79
1	C	217	LYS	CA-C	5.10	1.59	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455[A]	ASN	CA-C-N	8.30	136.64	121.70
1	B	455[A]	ASN	C-N-CA	8.30	136.64	121.70
1	B	455[B]	ASN	CA-C-N	8.30	136.64	121.70
1	B	455[B]	ASN	C-N-CA	8.30	136.64	121.70
1	C	154	ASP	CA-C-N	7.90	132.66	120.82
1	C	154	ASP	C-N-CA	7.90	132.66	120.82
1	B	239	GLU	CA-C-N	7.77	131.02	120.38
1	B	239	GLU	C-N-CA	7.77	131.02	120.38
1	C	411	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	411	ASP	CA-CB-CG	7.38	119.98	112.60
1	D	411	ASP	CA-CB-CG	7.38	119.98	112.60
1	B	411	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	289	THR	N-CA-C	-7.29	99.43	109.71
1	A	113	GLU	CB-CG-CD	7.08	124.63	112.60
1	B	113	GLU	CB-CG-CD	6.98	124.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	MET	CA-C-N	6.84	129.93	120.63
1	A	112	MET	C-N-CA	6.84	129.93	120.63
1	A	65	ARG	CA-C-N	6.64	129.07	120.44
1	A	65	ARG	C-N-CA	6.64	129.07	120.44
1	D	52	VAL	CA-C-N	6.58	130.45	121.05
1	D	52	VAL	C-N-CA	6.58	130.45	121.05
1	C	52	VAL	CA-C-N	6.50	130.34	121.05
1	C	52	VAL	C-N-CA	6.50	130.34	121.05
1	D	152	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	152	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	260	THR	CA-C-N	6.23	131.11	120.71
1	B	260	THR	C-N-CA	6.23	131.11	120.71
1	B	476	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	476	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	476	ASP	CA-CB-CG	6.12	118.72	112.60
1	C	456	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	66	SER	N-CA-C	6.04	117.87	111.28
1	C	152	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	152	ASP	CA-CB-CG	5.99	118.59	112.60
1	D	476	ASP	CA-CB-CG	5.95	118.55	112.60
1	D	78	GLY	CA-C-N	5.78	128.30	120.38
1	D	78	GLY	C-N-CA	5.78	128.30	120.38
1	A	342	VAL	N-CA-CB	5.76	115.44	110.08
1	B	342	VAL	N-CA-CB	5.75	115.43	110.08
1	C	463	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	65	ARG	CA-C-N	5.68	127.89	120.28
1	C	65	ARG	C-N-CA	5.68	127.89	120.28
1	D	155	GLU	CB-CG-CD	5.67	122.25	112.60
1	D	463	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	112	MET	CA-C-N	5.59	129.93	120.88
1	B	112	MET	C-N-CA	5.59	129.93	120.88
1	A	332	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	75	GLY	CA-C-N	5.55	128.28	120.28
1	B	75	GLY	C-N-CA	5.55	128.28	120.28
1	C	239	GLU	CA-C-N	5.41	127.79	120.38
1	C	239	GLU	C-N-CA	5.41	127.79	120.38
1	D	514	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	131	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	456	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	66	SER	N-CA-C	5.31	116.75	111.07
1	A	382	VAL	N-CA-CB	5.22	118.61	111.41
1	B	222	ASP	CA-CB-CG	5.16	117.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLY	CA-C-N	5.15	127.90	120.38
1	A	75	GLY	C-N-CA	5.15	127.90	120.38
1	A	158	ALA	N-CA-C	-5.12	105.78	111.36
1	B	463	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	153	ARG	CA-C-N	5.05	127.29	120.38
1	D	153	ARG	C-N-CA	5.05	127.29	120.38
1	C	75	GLY	CA-C-N	5.04	127.53	120.28
1	C	75	GLY	C-N-CA	5.04	127.53	120.28
1	A	239	GLU	CA-C-N	5.03	127.27	120.38
1	A	239	GLU	C-N-CA	5.03	127.27	120.38
1	A	514	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	118	TRP	CA-C-N	5.02	126.97	120.44
1	C	118	TRP	C-N-CA	5.02	126.97	120.44
1	C	333	GLU	CB-CG-CD	5.01	121.11	112.60

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	3858	0	3834	50	0
1	B	3857	0	3804	42	0
1	C	3900	0	3855	35	0
1	D	3893	0	3848	40	0
2	A	30	0	0	0	0
2	B	30	0	0	1	0
2	C	20	0	0	0	0
2	D	40	0	0	0	0
3	A	30	0	40	8	0
3	B	30	0	40	5	0
3	C	36	0	48	0	0
3	D	24	0	32	5	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	1	0
5	A	16	0	0	0	0
5	B	8	0	0	0	0
5	C	22	0	0	1	0
5	D	29	0	0	0	0
All	All	15846	0	15501	155	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 5.

All (155) 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:D:215:VAL:HG12	1:D:219:PHE:HE1	1.46	0.79
1:C:215:VAL:HG12	1:C:219:PHE:HE1	1.48	0.78
1:B:215:VAL:HG12	1:B:219:PHE:HE1	1.47	0.78
1:A:215:VAL:HG12	1:A:219:PHE:HE1	1.49	0.77
1:B:251:LYS:HG2	3:B:608:GOL:H12	1.74	0.68
1:A:321:LYS:HB2	3:A:609:GOL:H31	1.76	0.67
1:B:435:ARG:HH21	1:B:439:SER:HB3	1.59	0.66
1:B:461:GLU:HB2	1:C:469:ARG:HH12	1.61	0.65
1:B:261:ARG:HD3	1:B:271:TRP:CE2	2.32	0.64
1:B:91:GLN:HA	1:B:91:GLN:HE21	1.62	0.63
1:C:349:CYS:HB2	1:C:383:LEU:HD23	1.81	0.63
1:D:345:ASN:HD21	1:D:347:ALA:HB3	1.64	0.61
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.65	0.61
1:C:215:VAL:HG12	1:C:219:PHE:CE1	2.35	0.61
1:B:215:VAL:HG12	1:B:219:PHE:CE1	2.35	0.60
1:D:215:VAL:HG12	1:D:219:PHE:CE1	2.34	0.60
1:B:252:GLU:OE2	1:C:451:PRO:HA	2.00	0.60
1:A:60:VAL:HG13	1:A:65:ARG:HG3	1.83	0.60
1:D:253:MET:HE3	1:D:434:ILE:HG23	1.82	0.60
1:C:70:THR:HG21	1:C:164:ILE:HG23	1.84	0.59
3:A:608:GOL:H32	3:A:609:GOL:H2	1.85	0.59
1:D:349:CYS:HB2	1:D:383:LEU:HD23	1.83	0.59
1:B:415:GLN:HG2	1:B:429:ARG:HD3	1.85	0.58
1:A:252:GLU:N	3:A:610:GOL:H11	2.19	0.58
1:A:215:VAL:HG12	1:A:219:PHE:CE1	2.36	0.58
1:B:253:MET:HE1	1:B:466:TYR:CZ	2.40	0.57
1:B:475:PRO:HD3	1:C:452:GLY:HA2	1.86	0.57
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HG3	1:A:253:MET:HE2	1.87	0.56
1:D:181:LEU:HD21	1:D:214:ILE:HG13	1.86	0.56
1:B:449:LYS:HD2	1:B:455[B]:ASN:OD1	2.06	0.56
1:A:70:THR:HG21	1:A:164:ILE:HG23	1.88	0.55
1:C:91:GLN:HE21	1:C:91:GLN:HA	1.70	0.55
1:C:60:VAL:HG21	1:C:99:PRO:HA	1.89	0.55
1:A:253:MET:HE1	1:A:466:TYR:CZ	2.42	0.55
1:A:415:GLN:HG2	1:A:429:ARG:HD3	1.89	0.55
1:A:162:GLU:O	1:A:166:ARG:HG2	2.07	0.54
1:C:473:THR:HA	5:C:718:HOH:O	2.07	0.54
1:A:341:VAL:HG22	1:A:387:VAL:HG22	1.89	0.54
1:A:321:LYS:CB	3:A:609:GOL:H31	2.37	0.54
1:A:168:GLU:HG2	1:A:178:GLY:HA3	1.90	0.54
1:B:252:GLU:HG3	1:B:253:MET:HE2	1.89	0.54
1:C:278:CYS:SG	1:C:398:ILE:HD12	2.49	0.53
1:C:341:VAL:HG22	1:C:387:VAL:HG22	1.91	0.53
1:D:248:TYR:HA	1:D:251:LYS:HD2	1.89	0.53
1:B:352:GLY:HA2	1:B:521:LEU:O	2.09	0.53
1:D:62:PRO:HA	1:D:65:ARG:HG3	1.89	0.52
1:A:238:ASN:HB3	1:A:240:ARG:HE	1.75	0.52
1:C:352:GLY:HA2	1:C:521:LEU:O	2.10	0.52
1:A:253:MET:HE3	1:A:440:GLU:HB3	1.92	0.52
1:A:352:GLY:HA2	1:A:521:LEU:O	2.09	0.52
1:D:352:GLY:HA2	1:D:521:LEU:O	2.09	0.52
1:D:410:LEU:HD23	1:D:436:ALA:HB3	1.92	0.52
1:C:248:TYR:HA	1:C:251:LYS:HD2	1.91	0.51
1:A:248:TYR:HA	1:A:251:LYS:HD2	1.93	0.51
1:B:444:LEU:HD11	1:C:266:VAL:HG21	1.93	0.51
1:D:341:VAL:HG22	1:D:387:VAL:HG22	1.92	0.51
1:C:171:PHE:CE2	1:C:173:GLY:HA3	2.46	0.51
1:A:440:GLU:CG	3:A:610:GOL:H12	2.41	0.50
1:A:440:GLU:HG2	3:A:610:GOL:H12	1.93	0.50
1:D:258:ILE:HG21	3:D:609:GOL:H12	1.93	0.50
1:A:278:CYS:SG	1:A:398:ILE:HD12	2.51	0.50
1:A:306:ILE:HD13	1:A:383:LEU:CD1	2.41	0.50
1:D:305:VAL:HG22	3:D:612:GOL:C3	2.41	0.50
1:B:248:TYR:HA	1:B:251:LYS:HD2	1.93	0.50
1:B:457:THR:HG23	3:B:607:GOL:H11	1.93	0.50
1:A:306:ILE:HD13	1:A:383:LEU:HD11	1.94	0.50
1:A:62:PRO:HA	1:A:65:ARG:HD3	1.94	0.50
1:B:266:VAL:HG21	1:C:444:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HD3	1:A:175:GLU:HB3	1.93	0.49
1:C:435:ARG:HH21	1:C:439:SER:HB2	1.77	0.49
1:B:289:THR:HG21	1:B:365:TYR:HE1	1.77	0.48
1:D:79:ASP:HA	1:D:82:LYS:HE2	1.95	0.48
1:B:317:LEU:HD21	1:B:412:ILE:HG21	1.94	0.48
1:D:171:PHE:CE2	1:D:173:GLY:HA3	2.48	0.48
1:D:156:ASP:HA	1:D:159:ARG:HD3	1.96	0.48
1:D:248:TYR:CD2	1:D:309:HIS:HB3	2.49	0.48
1:C:253:MET:HE1	1:C:466:TYR:CZ	2.49	0.48
1:C:74:LEU:HD13	1:C:107:TYR:HB3	1.96	0.47
1:B:248:TYR:CD2	1:B:309:HIS:HB3	2.49	0.47
3:B:614:GOL:H11	1:D:390:ASP:HB3	1.97	0.47
1:A:248:TYR:CD2	1:A:309:HIS:HB3	2.50	0.47
1:C:248:TYR:CD2	1:C:309:HIS:HB3	2.49	0.47
1:D:305:VAL:HG22	3:D:612:GOL:H32	1.96	0.47
1:B:100:ARG:O	1:B:143:ARG:HD2	2.15	0.47
1:C:415:GLN:HG2	1:C:429:ARG:HD3	1.96	0.47
1:A:317:LEU:HD21	1:A:412:ILE:HG21	1.95	0.46
1:A:171:PHE:CE2	1:A:173:GLY:HA3	2.51	0.46
1:A:272:ASN:CB	1:A:391[B]:ARG:HG3	2.45	0.46
1:B:171:PHE:CE2	1:B:173:GLY:HA3	2.51	0.46
1:B:181:LEU:HD11	1:B:214:ILE:HD12	1.98	0.46
1:D:162:GLU:HA	1:D:165:LEU:HD12	1.97	0.46
1:C:112:MET:HG2	1:C:115:VAL:HG22	1.97	0.45
1:D:408:ARG:NH1	4:D:615:CL:CL	2.87	0.45
1:A:97:MET:HE1	1:D:453:LEU:HD13	1.97	0.45
1:A:179:ASN:HD22	1:A:210:TRP:H	1.63	0.45
1:A:489:ASN:OD1	1:A:491:THR:HG23	2.16	0.45
1:B:215:VAL:CG1	1:B:219:PHE:HE1	2.25	0.45
1:B:544:THR:HG22	1:B:545:THR:H	1.82	0.45
1:D:60:VAL:HG13	1:D:65:ARG:HG2	1.99	0.45
1:D:210:TRP:CB	3:D:610:GOL:H2	2.47	0.45
1:D:215:VAL:CG1	1:D:219:PHE:HE1	2.25	0.45
1:D:277:ALA:O	1:D:396:PRO:HD2	2.16	0.45
1:D:210:TRP:HB3	3:D:610:GOL:H2	1.99	0.45
1:C:62:PRO:HA	1:C:65:ARG:HG3	1.99	0.44
1:C:450:THR:HG22	1:C:458:HIS:HB3	1.99	0.44
1:A:475:PRO:HD3	1:D:452:GLY:HA2	1.98	0.44
1:C:67:ARG:HG2	1:C:178:GLY:HA2	2.00	0.44
1:D:67:ARG:HG2	1:D:178:GLY:HA2	2.00	0.44
1:D:450:THR:HG22	1:D:458:HIS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:VAL:HG12	1:B:400:ARG:HG2	2.00	0.43
3:A:607:GOL:H11	1:C:391:ARG:HA	1.98	0.43
1:A:382:VAL:HG12	1:A:400:ARG:HG2	1.99	0.43
1:B:70:THR:HG21	1:B:164:ILE:HG23	2.00	0.43
1:B:289:THR:HG21	1:B:365:TYR:CE1	2.53	0.43
1:C:327:ALA:HA	1:C:491:THR:HG23	2.00	0.43
1:D:278:CYS:SG	1:D:398:ILE:HD12	2.59	0.43
1:B:444:LEU:HD21	1:C:266:VAL:HG11	2.01	0.43
1:C:277:ALA:O	1:C:396:PRO:HD2	2.18	0.43
1:D:115:VAL:O	1:D:119:LYS:HG3	2.18	0.43
1:A:266:VAL:HG11	1:D:444:LEU:HD21	2.01	0.43
1:B:159:ARG:HD2	2:B:604:SO4:O1	2.18	0.43
1:A:272:ASN:HB3	1:A:391[B]:ARG:HG3	2.01	0.42
1:B:102:VAL:O	1:B:143:ARG:HD3	2.19	0.42
1:A:238:ASN:HD22	1:A:240:ARG:NH2	2.18	0.42
1:A:74:LEU:HB3	1:A:186:LEU:HD21	2.01	0.42
1:A:410:LEU:HD23	1:A:436:ALA:HB3	2.01	0.42
1:D:98:LEU:HB3	1:D:102:VAL:HG21	2.00	0.42
1:A:350:VAL:HB	1:A:382:VAL:HG22	2.01	0.42
1:B:251:LYS:HZ2	3:B:608:GOL:H32	1.85	0.42
1:B:277:ALA:O	1:B:396:PRO:HD2	2.19	0.42
1:A:414:ILE:HD13	1:A:432:LEU:HD23	2.01	0.41
1:B:64:LEU:HD21	1:B:486:LEU:HB3	2.02	0.41
1:A:453:LEU:HD23	1:D:97:MET:SD	2.60	0.41
1:B:181:LEU:HD21	1:B:214:ILE:HG13	2.00	0.41
1:A:277:ALA:O	1:A:396:PRO:HD2	2.20	0.41
1:B:450:THR:OG1	1:B:456:ASP:HB3	2.20	0.41
1:C:247:HIS:HA	1:C:481:LEU:HD11	2.02	0.41
1:A:150:SER:OG	1:A:153:ARG:HB2	2.20	0.41
1:C:292:ARG:HA	1:C:292:ARG:HD3	1.94	0.41
1:D:69:LEU:HD23	1:D:102:VAL:HG13	2.02	0.41
1:D:161:ASN:O	1:D:165:LEU:HG	2.20	0.41
1:A:107:TYR:CD2	1:A:160:LEU:HD13	2.55	0.41
1:A:251:LYS:HZ2	3:A:611:GOL:H12	1.86	0.41
1:A:417:LYS:HB2	1:D:265:ARG:HD2	2.02	0.41
1:A:444:LEU:HD11	1:D:266:VAL:HG21	2.02	0.41
1:B:450:THR:HG22	1:B:458:HIS:HB3	2.03	0.40
1:D:350:VAL:HB	1:D:382:VAL:HG13	2.03	0.40
1:C:350:VAL:HB	1:C:382:VAL:HG13	2.03	0.40
1:A:215:VAL:CG1	1:A:219:PHE:HE1	2.26	0.40
1:A:328[A]:GLU:OE1	1:A:328[A]:GLU:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD13	1:B:107:TYR:HB3	2.04	0.40
1:B:210:TRP:HA	3:B:609:GOL:H2	2.02	0.40
1:B:475:PRO:CD	1:C:452:GLY:HA2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/541 (90%)	462 (95%)	25 (5%)	1 (0%)	43	62
1	B	489/541 (90%)	456 (93%)	30 (6%)	3 (1%)	21	38
1	C	495/541 (92%)	469 (95%)	25 (5%)	1 (0%)	43	62
1	D	494/541 (91%)	469 (95%)	24 (5%)	1 (0%)	43	62
All	All	1966/2164 (91%)	1856 (94%)	104 (5%)	6 (0%)	36	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	GLU
1	B	290	GLU
1	B	440	GLU
1	B	456	ASP
1	C	174	PRO
1	D	174	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	412/462 (89%)	387 (94%)	25 (6%)	17	35
1	B	412/462 (89%)	381 (92%)	31 (8%)	12	26
1	C	417/462 (90%)	384 (92%)	33 (8%)	11	24
1	D	416/462 (90%)	384 (92%)	32 (8%)	12	25
All	All	1657/1848 (90%)	1536 (93%)	121 (7%)	14	27

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	MET
1	A	113	GLU
1	A	133	ARG
1	A	135	CYS
1	A	145	SER
1	A	186	LEU
1	A	205	LYS
1	A	211	VAL
1	A	213	LEU
1	A	217	LYS
1	A	233	LEU
1	A	240	ARG
1	A	245	ILE
1	A	268	SER
1	A	285	GLU
1	A	328[A]	GLU
1	A	328[B]	GLU
1	A	342	VAL
1	A	345	ASN
1	A	418	ASP
1	A	421	ARG
1	A	474	LEU
1	A	491	THR
1	A	539	ILE
1	A	544	THR
1	B	63	GLU
1	B	79	ASP
1	B	91	GLN
1	B	97	MET
1	B	113	GLU

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Mol	Chain	Res	Type
1	B	145	SER
1	B	163	ARG
1	B	181	LEU
1	B	186	LEU
1	B	213	LEU
1	B	217	LYS
1	B	228	GLN
1	B	233	LEU
1	B	245	ILE
1	B	268	SER
1	B	285	GLU
1	B	290	GLU
1	B	295	TYR
1	B	328	GLU
1	B	339	ARG
1	B	345	ASN
1	B	361	SER
1	B	418	ASP
1	B	453	LEU
1	B	454	LEU
1	B	455[A]	ASN
1	B	455[B]	ASN
1	B	456	ASP
1	B	459	GLN
1	B	491	THR
1	B	539	ILE
1	C	61	SER
1	C	70	THR
1	C	79	ASP
1	C	91	GLN
1	C	102	VAL
1	C	110	SER
1	C	112	MET
1	C	113	GLU
1	C	145	SER
1	C	176	LYS
1	C	186	LEU
1	C	190	VAL
1	C	213	LEU
1	C	228[A]	GLN
1	C	228[B]	GLN
1	C	233	LEU

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Mol	Chain	Res	Type
1	C	245	ILE
1	C	252	GLU
1	C	268	SER
1	C	285	GLU
1	C	287	ILE
1	C	317	LEU
1	C	328	GLU
1	C	345	ASN
1	C	376	HIS
1	C	382	VAL
1	C	418[A]	ASP
1	C	418[B]	ASP
1	C	453	LEU
1	C	459	GLN
1	C	474	LEU
1	C	491	THR
1	C	539	ILE
1	D	61	SER
1	D	79	ASP
1	D	82	LYS
1	D	102	VAL
1	D	112	MET
1	D	145	SER
1	D	166	ARG
1	D	181	LEU
1	D	186	LEU
1	D	213	LEU
1	D	217	LYS
1	D	233	LEU
1	D	245	ILE
1	D	268	SER
1	D	285	GLU
1	D	289	THR
1	D	290	GLU
1	D	295	TYR
1	D	317	LEU
1	D	320	GLU
1	D	328	GLU
1	D	345	ASN
1	D	382	VAL
1	D	418[A]	ASP
1	D	418[B]	ASP

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Mol	Chain	Res	Type
1	D	421	ARG
1	D	453	LEU
1	D	459	GLN
1	D	474	LEU
1	D	491	THR
1	D	539	ILE
1	D	544	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	231	ASN
1	A	238	ASN
1	A	309	HIS
1	A	345	ASN
1	A	492	ASN
1	B	91	GLN
1	B	136	HIS
1	B	179	ASN
1	B	228	GLN
1	B	238	ASN
1	B	309	HIS
1	B	386	HIS
1	B	388	ASN
1	B	492	ASN
1	C	91	GLN
1	C	172	GLN
1	C	232	GLN
1	C	241	GLN
1	C	255	GLN
1	D	139	ASN
1	D	255	GLN
1	D	345	ASN
1	D	492	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 23 are monoatomic - leaving 44 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	607	-	5,5,5	0.21	0	5,5,5	0.44	0
3	GOL	B	615	-	5,5,5	0.24	0	5,5,5	0.22	0
3	GOL	C	611	-	5,5,5	0.14	0	5,5,5	0.26	0
3	GOL	C	602	-	5,5,5	0.18	0	5,5,5	0.37	0
2	SO4	D	604	-	4,4,4	0.21	0	6,6,6	0.21	0
3	GOL	B	614	-	5,5,5	0.19	0	5,5,5	0.24	0
2	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.15	0
3	GOL	C	601	-	5,5,5	0.14	0	5,5,5	0.25	0
2	SO4	C	606	-	4,4,4	0.51	0	6,6,6	0.32	0
2	SO4	D	602	-	4,4,4	0.30	0	6,6,6	0.22	0
3	GOL	A	609	-	5,5,5	0.12	0	5,5,5	0.25	0
2	SO4	C	605	-	4,4,4	0.33	0	6,6,6	0.20	0
2	SO4	D	601	-	4,4,4	0.35	0	6,6,6	0.31	0
3	GOL	B	609	-	5,5,5	0.15	0	5,5,5	0.28	0
3	GOL	C	610	-	5,5,5	0.30	0	5,5,5	0.34	0
3	GOL	A	607	-	5,5,5	0.20	0	5,5,5	0.84	0
2	SO4	D	603	-	4,4,4	0.30	0	6,6,6	0.29	0
2	SO4	D	605	-	4,4,4	0.29	0	6,6,6	0.12	0
2	SO4	C	604	-	4,4,4	0.34	0	6,6,6	0.49	0
2	SO4	C	607	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	B	606	-	4,4,4	0.28	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	604	-	4,4,4	0.32	0	6,6,6	0.14	0
3	GOL	C	609	-	5,5,5	0.16	0	5,5,5	0.31	0
2	SO4	D	606	-	4,4,4	0.27	0	6,6,6	0.13	0
3	GOL	C	608	-	5,5,5	0.11	0	5,5,5	0.40	0
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.51	0
2	SO4	D	607	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	B	604	-	4,4,4	0.48	0	6,6,6	0.29	0
3	GOL	D	611	-	5,5,5	0.22	0	5,5,5	0.23	0
2	SO4	A	601	-	4,4,4	0.31	0	6,6,6	0.38	0
3	GOL	A	610	-	5,5,5	0.13	0	5,5,5	0.99	0
3	GOL	D	609	-	5,5,5	0.20	0	5,5,5	0.50	0
2	SO4	A	602	-	4,4,4	0.40	0	6,6,6	0.32	0
2	SO4	B	602	-	4,4,4	0.37	0	6,6,6	0.35	0
3	GOL	A	611	-	5,5,5	0.11	0	5,5,5	0.41	0
2	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	D	608	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	A	606	-	4,4,4	0.31	0	6,6,6	0.25	0
2	SO4	B	603	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	A	608	-	5,5,5	0.15	0	5,5,5	0.38	0
3	GOL	D	610	-	5,5,5	0.21	0	5,5,5	0.59	0
3	GOL	D	612	-	5,5,5	0.13	0	5,5,5	0.21	0
3	GOL	B	608	-	5,5,5	0.20	0	5,5,5	0.30	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	GOL	B	607	-	-	1/4/4/4	-
3	GOL	B	615	-	-	2/4/4/4	-
3	GOL	C	611	-	-	0/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	B	614	-	-	2/4/4/4	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	A	609	-	-	2/4/4/4	-
3	GOL	B	609	-	-	0/4/4/4	-
3	GOL	C	610	-	-	0/4/4/4	-
3	GOL	A	607	-	-	0/4/4/4	-
3	GOL	C	609	-	-	0/4/4/4	-
3	GOL	C	608	-	-	1/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	609	-	-	0/4/4/4	-
3	GOL	A	610	-	-	2/4/4/4	-
3	GOL	A	611	-	-	0/4/4/4	-
3	GOL	A	608	-	-	2/4/4/4	-
3	GOL	D	610	-	-	2/4/4/4	-
3	GOL	D	612	-	-	2/4/4/4	-
3	GOL	D	611	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	609	GOL	O1-C1-C2-C3
3	B	608	GOL	C1-C2-C3-O3
3	B	615	GOL	O1-C1-C2-C3
3	D	610	GOL	C1-C2-C3-O3
3	D	611	GOL	O1-C1-C2-O2
3	D	612	GOL	C1-C2-C3-O3
3	A	609	GOL	O1-C1-C2-O2
3	A	608	GOL	C1-C2-C3-O3
3	A	610	GOL	C1-C2-C3-O3
3	D	611	GOL	O1-C1-C2-C3
3	D	611	GOL	C1-C2-C3-O3
3	D	610	GOL	O2-C2-C3-O3
3	D	612	GOL	O2-C2-C3-O3
3	B	608	GOL	O2-C2-C3-O3
3	A	610	GOL	O2-C2-C3-O3
3	B	615	GOL	O1-C1-C2-O2
3	A	608	GOL	O2-C2-C3-O3
3	D	611	GOL	O2-C2-C3-O3
3	C	608	GOL	C1-C2-C3-O3
3	B	614	GOL	O1-C1-C2-C3
3	B	614	GOL	O1-C1-C2-O2
3	B	607	GOL	C1-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	607	GOL	1	0
3	B	614	GOL	1	0
3	A	609	GOL	3	0
3	B	609	GOL	1	0
3	A	607	GOL	1	0
2	B	604	SO4	1	0
3	A	610	GOL	3	0
3	D	609	GOL	1	0
3	A	611	GOL	1	0
3	A	608	GOL	1	0
3	D	610	GOL	2	0
3	D	612	GOL	2	0
3	B	608	GOL	2	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, 95th 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 ²)	Q<0.9
1	A	487/541 (90%)	0.37	24 (4%) 35 27	7, 44, 82, 106	3 (0%)
1	B	490/541 (90%)	0.25	14 (2%) 53 45	14, 41, 78, 99	1 (0%)
1	C	494/541 (91%)	0.40	24 (4%) 35 27	13, 41, 78, 98	3 (0%)
1	D	494/541 (91%)	0.30	20 (4%) 42 33	13, 41, 75, 99	2 (0%)
All	All	1965/2164 (90%)	0.33	82 (4%) 40 32	7, 42, 79, 106	9 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	TYR	5.3
1	D	295	TYR	4.5
1	C	52	VAL	4.4
1	D	146	TYR	4.3
1	B	295	TYR	3.9
1	C	470	TYR	3.8
1	A	545	THR	3.8
1	A	473	THR	3.8
1	B	455[A]	ASN	3.7
1	C	473	THR	3.4
1	C	188	PRO	3.4
1	C	293	GLY	3.3
1	C	466	TYR	3.2
1	C	440	GLU	3.1
1	C	376	HIS	3.1
1	A	369	PRO	3.1
1	B	131	ASP	3.0
1	D	545	THR	3.0
1	A	206	PRO	3.0
1	A	132	GLU	3.0
1	D	293	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	187	PRO	3.0
1	A	295	TYR	2.9
1	A	176	LYS	2.9
1	B	369	PRO	2.8
1	C	142[A]	ARG	2.8
1	D	465	THR	2.8
1	A	373	LYS	2.8
1	B	57	PRO	2.8
1	D	52	VAL	2.8
1	A	534	GLN	2.7
1	B	172	GLN	2.7
1	A	94	CYS	2.7
1	C	176	LYS	2.7
1	C	289	THR	2.6
1	A	197	GLY	2.6
1	C	113	GLU	2.6
1	A	172	GLN	2.6
1	A	133	ARG	2.5
1	D	157	PHE	2.5
1	D	201	GLY	2.5
1	D	473	THR	2.5
1	C	291	GLY	2.5
1	C	461	GLU	2.5
1	D	292	ARG	2.5
1	C	545	THR	2.5
1	A	130	LEU	2.4
1	B	56	ILE	2.4
1	B	132	GLU	2.4
1	C	469	ARG	2.4
1	D	290	GLU	2.4
1	B	58	ASP	2.4
1	B	291	GLY	2.4
1	D	188	PRO	2.4
1	A	131	ASP	2.4
1	D	112	MET	2.4
1	D	470	TYR	2.4
1	A	360	GLY	2.3
1	D	358	ALA	2.3
1	D	289	THR	2.3
1	D	467	GLU	2.3
1	D	335	VAL	2.3
1	C	373	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	294	GLY	2.3
1	B	360	GLY	2.2
1	C	112	MET	2.2
1	C	253	MET	2.2
1	A	525	ALA	2.2
1	A	202	ALA	2.2
1	B	130	LEU	2.2
1	A	129	ARG	2.2
1	A	135	CYS	2.2
1	B	376	HIS	2.1
1	B	373	LYS	2.1
1	A	125	GLY	2.1
1	A	128	THR	2.1
1	D	466	TYR	2.1
1	C	465	THR	2.1
1	C	533	ALA	2.1
1	A	177	GLY	2.0
1	A	201	GLY	2.0
1	C	189	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	GOL	B	609	6/6	0.58	0.25	72,78,82,84	0
2	SO4	D	604	5/5	0.61	0.23	90,92,92,94	0
2	SO4	A	605	5/5	0.66	0.23	106,107,107,108	0
4	CL	B	611	1/1	0.66	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	603	5/5	0.67	0.24	121,121,122,123	0
3	GOL	C	611	6/6	0.68	0.18	56,60,61,64	0
3	GOL	A	610	6/6	0.68	0.26	51,54,55,56	0
3	GOL	A	608	6/6	0.71	0.19	55,57,58,59	0
3	GOL	D	612	6/6	0.72	0.18	59,62,63,64	0
2	SO4	D	608	5/5	0.72	0.19	104,105,106,108	0
3	GOL	D	610	6/6	0.74	0.21	37,53,55,55	0
3	GOL	A	607	6/6	0.75	0.19	38,43,46,46	0
2	SO4	D	603	5/5	0.75	0.20	72,72,74,77	0
3	GOL	B	615	6/6	0.76	0.18	40,48,49,49	0
3	GOL	C	610	6/6	0.76	0.15	46,51,52,52	0
2	SO4	C	607	5/5	0.76	0.15	105,105,106,107	0
3	GOL	C	601	6/6	0.77	0.26	73,75,77,77	0
2	SO4	D	605	5/5	0.78	0.16	123,123,123,123	0
3	GOL	D	609	6/6	0.79	0.20	51,56,58,59	0
4	CL	D	615	1/1	0.80	0.18	77,77,77,77	0
3	GOL	B	608	6/6	0.81	0.15	50,56,58,59	0
2	SO4	C	606	5/5	0.83	0.18	69,75,75,76	0
3	GOL	A	611	6/6	0.83	0.14	53,56,61,62	0
3	GOL	B	607	6/6	0.83	0.15	43,45,47,47	0
3	GOL	C	602	6/6	0.83	0.15	42,42,43,44	0
3	GOL	C	609	6/6	0.83	0.13	42,46,49,49	0
4	CL	C	603	1/1	0.83	0.16	79,79,79,79	0
3	GOL	A	609	6/6	0.83	0.19	55,60,60,61	0
4	CL	A	615	1/1	0.84	0.12	68,68,68,68	0
2	SO4	D	607	5/5	0.85	0.22	107,108,108,109	0
3	GOL	C	608	6/6	0.85	0.12	44,45,45,47	0
4	CL	D	616	1/1	0.85	0.12	82,82,82,82	0
4	CL	B	612	1/1	0.86	0.13	67,67,67,67	0
2	SO4	D	602	5/5	0.86	0.15	79,80,83,83	0
4	CL	C	614	1/1	0.87	0.12	68,68,68,68	0
2	SO4	A	603	5/5	0.88	0.11	69,72,72,74	0
4	CL	C	615	1/1	0.88	0.10	68,68,68,68	0
4	CL	D	617	1/1	0.88	0.10	66,66,66,66	0
2	SO4	A	604	5/5	0.89	0.15	67,68,68,70	0
3	GOL	D	611	6/6	0.89	0.11	31,34,39,45	0
2	SO4	B	604	5/5	0.89	0.09	59,62,64,65	0
2	SO4	C	605	5/5	0.89	0.15	70,71,72,72	0
2	SO4	B	602	5/5	0.90	0.11	68,68,70,70	0
4	CL	A	616	1/1	0.90	0.10	59,59,59,59	0
4	CL	C	618	1/1	0.90	0.13	57,57,57,57	0
2	SO4	B	606	5/5	0.90	0.31	106,107,107,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	602	5/5	0.90	0.11	68,69,69,71	0
4	CL	A	614	1/1	0.90	0.12	74,74,74,74	0
4	CL	C	619	1/1	0.91	0.11	67,67,67,67	0
4	CL	A	612	1/1	0.91	0.10	58,58,58,58	0
4	CL	C	616	1/1	0.91	0.13	80,80,80,80	0
2	SO4	B	601	5/5	0.91	0.10	49,50,52,57	0
2	SO4	A	601	5/5	0.93	0.09	55,56,57,62	0
3	GOL	B	614	6/6	0.93	0.10	23,29,33,37	0
4	CL	C	612	1/1	0.94	0.06	48,48,48,48	0
4	CL	C	613	1/1	0.94	0.12	64,64,64,64	0
4	CL	C	617	1/1	0.94	0.21	67,67,67,67	0
2	SO4	D	606	5/5	0.94	0.27	130,131,131,132	0
4	CL	D	614	1/1	0.95	0.07	69,69,69,69	0
4	CL	B	610	1/1	0.95	0.10	60,60,60,60	0
2	SO4	D	601	5/5	0.95	0.08	40,43,45,46	0
4	CL	D	613	1/1	0.95	0.09	67,67,67,67	0
2	SO4	C	604	5/5	0.96	0.07	42,43,44,46	0
4	CL	A	613	1/1	0.97	0.05	41,41,41,41	0
4	CL	B	613	1/1	0.97	0.08	47,47,47,47	0
2	SO4	A	606	5/5	0.97	0.07	44,45,48,52	0
2	SO4	B	605	5/5	0.97	0.07	43,44,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.