



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:05 PM UTC

PDB ID : 2B4K / pdb_00002b4k
Title : Acetobacter turbidans alpha-amino acid ester hydrolase complexed with phenylglycine
Authors : Barends, T.R.M.; Polderman-Tijmes, J.J.; Jekel, P.A.; Williams, C.; Wybenga, G.; Janssen, D.B.; Dijkstra, B.W.
Deposited on : 2005-09-26
Resolution : 3.30 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

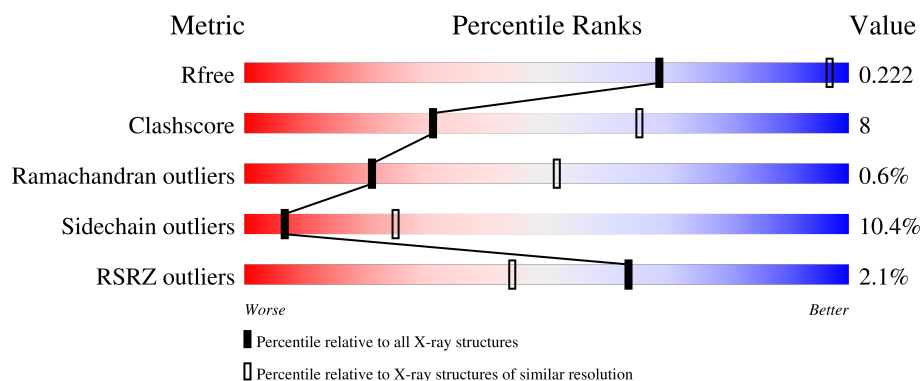
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	652	
1	B	652	
1	C	652	
1	D	652	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19594 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 Alpha-amino acid ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			4883	3111	845	907	20			
1	B	617	Total	C	N	O	S	0	0	0
			4883	3111	845	907	20			
1	C	617	Total	C	N	O	S	0	0	0
			4883	3111	845	907	20			
1	D	617	Total	C	N	O	S	0	0	0
			4883	3111	845	907	20			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LYS	-	expression tag	UNP Q8VRK8
A	669	LEU	-	expression tag	UNP Q8VRK8
A	670	GLY	-	expression tag	UNP Q8VRK8
A	671	PRO	-	expression tag	UNP Q8VRK8
A	672	GLU	-	expression tag	UNP Q8VRK8
A	673	GLN	-	expression tag	UNP Q8VRK8
A	674	LYS	-	expression tag	UNP Q8VRK8
A	675	LEU	-	expression tag	UNP Q8VRK8
A	676	ILE	-	expression tag	UNP Q8VRK8
A	677	SER	-	expression tag	UNP Q8VRK8
A	678	GLU	-	expression tag	UNP Q8VRK8
A	679	GLU	-	expression tag	UNP Q8VRK8
A	680	ASP	-	expression tag	UNP Q8VRK8
A	681	LEU	-	expression tag	UNP Q8VRK8
A	682	ASN	-	expression tag	UNP Q8VRK8
A	683	SER	-	expression tag	UNP Q8VRK8
A	684	ALA	-	expression tag	UNP Q8VRK8
A	685	VAL	-	expression tag	UNP Q8VRK8
A	686	ASP	-	expression tag	UNP Q8VRK8
A	687	HIS	-	expression tag	UNP Q8VRK8
A	688	HIS	-	expression tag	UNP Q8VRK8

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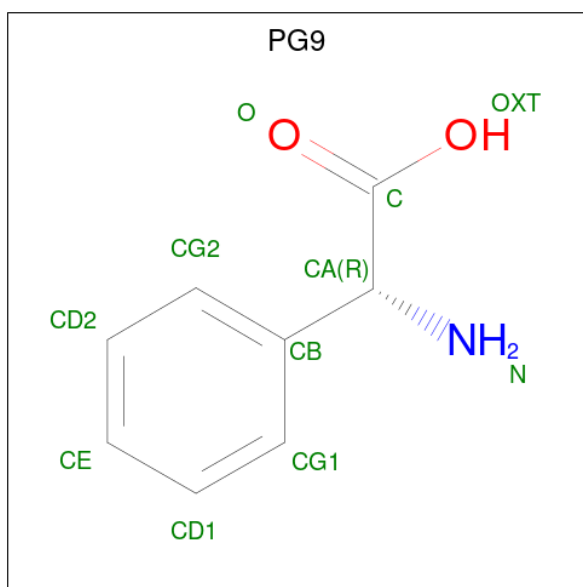
Chain	Residue	Modelled	Actual	Comment	Reference
A	689	HIS	-	expression tag	UNP Q8VRK8
A	690	HIS	-	expression tag	UNP Q8VRK8
A	691	HIS	-	expression tag	UNP Q8VRK8
A	692	HIS	-	expression tag	UNP Q8VRK8
B	668	LYS	-	expression tag	UNP Q8VRK8
B	669	LEU	-	expression tag	UNP Q8VRK8
B	670	GLY	-	expression tag	UNP Q8VRK8
B	671	PRO	-	expression tag	UNP Q8VRK8
B	672	GLU	-	expression tag	UNP Q8VRK8
B	673	GLN	-	expression tag	UNP Q8VRK8
B	674	LYS	-	expression tag	UNP Q8VRK8
B	675	LEU	-	expression tag	UNP Q8VRK8
B	676	ILE	-	expression tag	UNP Q8VRK8
B	677	SER	-	expression tag	UNP Q8VRK8
B	678	GLU	-	expression tag	UNP Q8VRK8
B	679	GLU	-	expression tag	UNP Q8VRK8
B	680	ASP	-	expression tag	UNP Q8VRK8
B	681	LEU	-	expression tag	UNP Q8VRK8
B	682	ASN	-	expression tag	UNP Q8VRK8
B	683	SER	-	expression tag	UNP Q8VRK8
B	684	ALA	-	expression tag	UNP Q8VRK8
B	685	VAL	-	expression tag	UNP Q8VRK8
B	686	ASP	-	expression tag	UNP Q8VRK8
B	687	HIS	-	expression tag	UNP Q8VRK8
B	688	HIS	-	expression tag	UNP Q8VRK8
B	689	HIS	-	expression tag	UNP Q8VRK8
B	690	HIS	-	expression tag	UNP Q8VRK8
B	691	HIS	-	expression tag	UNP Q8VRK8
B	692	HIS	-	expression tag	UNP Q8VRK8
C	668	LYS	-	expression tag	UNP Q8VRK8
C	669	LEU	-	expression tag	UNP Q8VRK8
C	670	GLY	-	expression tag	UNP Q8VRK8
C	671	PRO	-	expression tag	UNP Q8VRK8
C	672	GLU	-	expression tag	UNP Q8VRK8
C	673	GLN	-	expression tag	UNP Q8VRK8
C	674	LYS	-	expression tag	UNP Q8VRK8
C	675	LEU	-	expression tag	UNP Q8VRK8
C	676	ILE	-	expression tag	UNP Q8VRK8
C	677	SER	-	expression tag	UNP Q8VRK8
C	678	GLU	-	expression tag	UNP Q8VRK8
C	679	GLU	-	expression tag	UNP Q8VRK8
C	680	ASP	-	expression tag	UNP Q8VRK8

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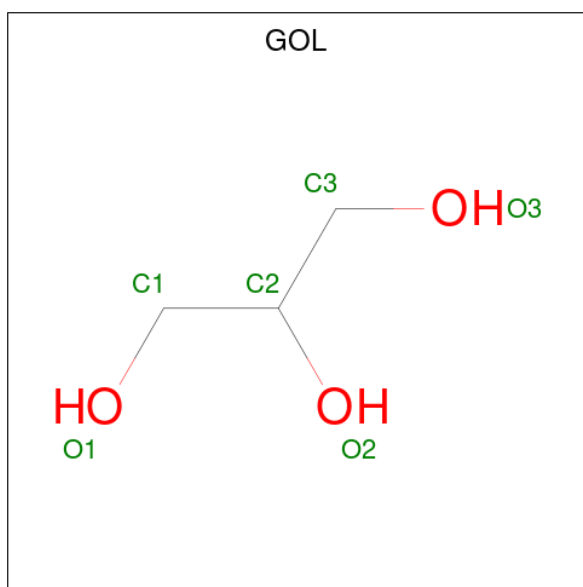
Chain	Residue	Modelled	Actual	Comment	Reference
C	681	LEU	-	expression tag	UNP Q8VRK8
C	682	ASN	-	expression tag	UNP Q8VRK8
C	683	SER	-	expression tag	UNP Q8VRK8
C	684	ALA	-	expression tag	UNP Q8VRK8
C	685	VAL	-	expression tag	UNP Q8VRK8
C	686	ASP	-	expression tag	UNP Q8VRK8
C	687	HIS	-	expression tag	UNP Q8VRK8
C	688	HIS	-	expression tag	UNP Q8VRK8
C	689	HIS	-	expression tag	UNP Q8VRK8
C	690	HIS	-	expression tag	UNP Q8VRK8
C	691	HIS	-	expression tag	UNP Q8VRK8
C	692	HIS	-	expression tag	UNP Q8VRK8
D	668	LYS	-	expression tag	UNP Q8VRK8
D	669	LEU	-	expression tag	UNP Q8VRK8
D	670	GLY	-	expression tag	UNP Q8VRK8
D	671	PRO	-	expression tag	UNP Q8VRK8
D	672	GLU	-	expression tag	UNP Q8VRK8
D	673	GLN	-	expression tag	UNP Q8VRK8
D	674	LYS	-	expression tag	UNP Q8VRK8
D	675	LEU	-	expression tag	UNP Q8VRK8
D	676	ILE	-	expression tag	UNP Q8VRK8
D	677	SER	-	expression tag	UNP Q8VRK8
D	678	GLU	-	expression tag	UNP Q8VRK8
D	679	GLU	-	expression tag	UNP Q8VRK8
D	680	ASP	-	expression tag	UNP Q8VRK8
D	681	LEU	-	expression tag	UNP Q8VRK8
D	682	ASN	-	expression tag	UNP Q8VRK8
D	683	SER	-	expression tag	UNP Q8VRK8
D	684	ALA	-	expression tag	UNP Q8VRK8
D	685	VAL	-	expression tag	UNP Q8VRK8
D	686	ASP	-	expression tag	UNP Q8VRK8
D	687	HIS	-	expression tag	UNP Q8VRK8
D	688	HIS	-	expression tag	UNP Q8VRK8
D	689	HIS	-	expression tag	UNP Q8VRK8
D	690	HIS	-	expression tag	UNP Q8VRK8
D	691	HIS	-	expression tag	UNP Q8VRK8
D	692	HIS	-	expression tag	UNP Q8VRK8

- Molecule 2 is D-PHENYLGLYCINE (CCD ID: PG9) (formula: $C_8H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	8	1	2		
2	B	1	Total	C	N	O	0	0
			11	8	1	2		
2	D	1	Total	C	N	O	0	0
			11	8	1	2		

- 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	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

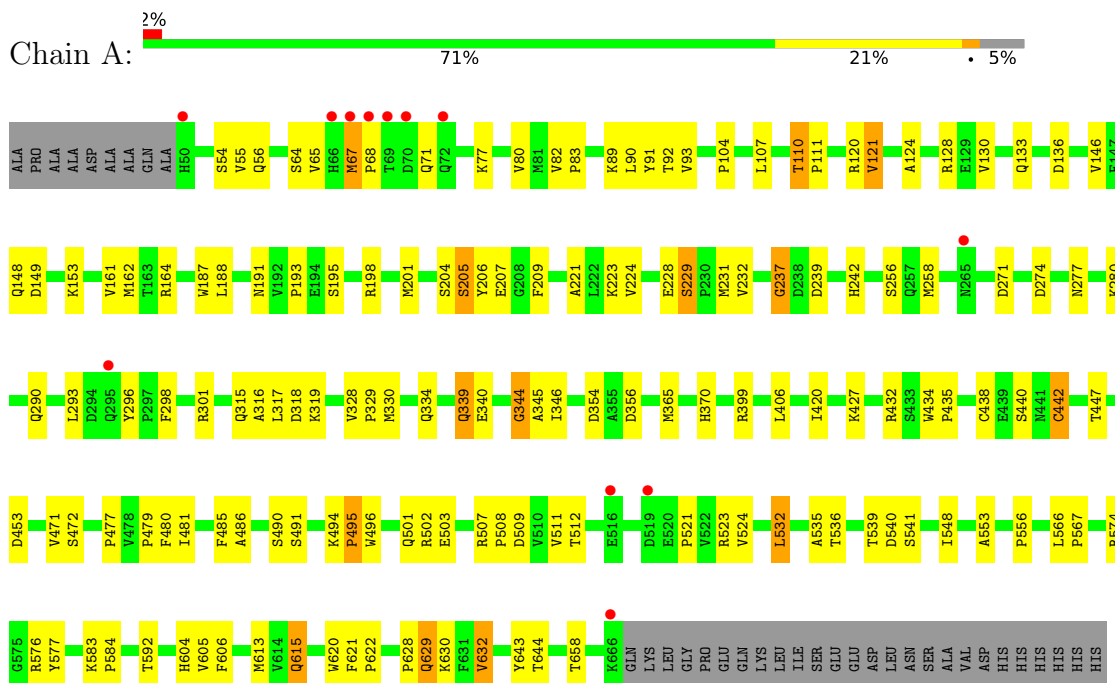
- Molecule 4 is water.

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

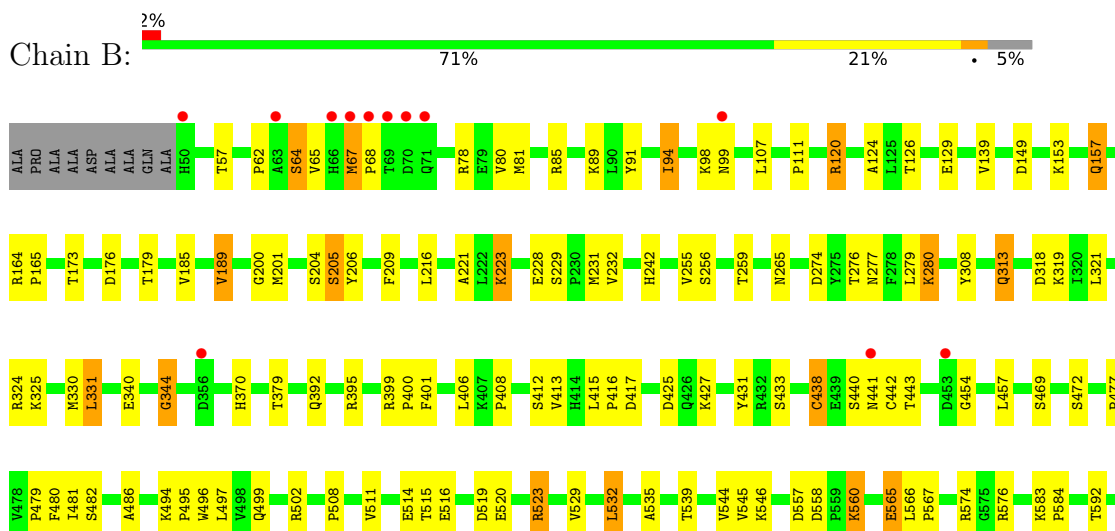
3 Residue-property plots [i](#)

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: Alpha-amino acid ester hydrolase



• Molecule 1: Alpha-amino acid ester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	340.91Å 340.91Å 340.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (15.00-3.30) 98.2 (15.00-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.258 , 0.289 0.221 , 0.222	Depositor DCC
R_{free} test set	4721 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19594	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG9

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	0.54	0/5042	0.87	2/6887 (0.0%)
1	B	0.54	0/5042	0.87	2/6887 (0.0%)
1	C	0.54	1/5042 (0.0%)	0.86	1/6887 (0.0%)
1	D	0.53	1/5042 (0.0%)	0.88	5/6887 (0.1%)
All	All	0.54	2/20168 (0.0%)	0.87	10/27548 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	MET	SD-CE	5.32	1.92	1.79
1	D	67	MET	SD-CE	5.18	1.92	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	VAL	N-CA-C	-6.56	101.66	108.15
1	B	139	VAL	N-CA-C	-5.79	104.69	111.00
1	D	275	TYR	N-CA-C	-5.71	104.96	111.07
1	B	454	GLY	N-CA-C	-5.62	107.44	115.64
1	D	317	LEU	N-CA-C	5.59	118.10	111.33
1	C	275	TYR	N-CA-C	-5.38	105.31	111.07
1	A	532	LEU	N-CA-C	5.33	117.42	108.73
1	D	139	VAL	N-CA-C	-5.20	105.33	111.00
1	D	121	VAL	N-CA-C	-5.06	103.14	108.15
1	D	519	ASP	N-CA-C	-5.03	107.32	113.50

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	4883	0	4648	78	0
1	B	4883	0	4648	80	0
1	C	4883	0	4648	80	0
1	D	4883	0	4648	85	0
2	A	11	0	8	1	0
2	B	11	0	8	1	0
2	D	11	0	8	4	0
3	A	12	0	16	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
All	All	19594	0	18648	312	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 8.

All (312) 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:438:CYS:HG	1:A:442:CYS:HG	1.07	0.95
1:D:232:VAL:HB	1:D:344:GLY:HA2	1.56	0.87
1:C:70:ASP:HA	1:C:73:ARG:HD2	1.57	0.85
1:D:205:SER:OG	1:D:206:TYR:N	2.09	0.84
1:C:482:SER:O	1:C:492:ARG:NH1	2.11	0.83
1:B:232:VAL:HB	1:B:344:GLY:HA2	1.66	0.78
1:B:205:SER:OG	1:B:370:HIS:NE2	2.19	0.76
1:A:501:GLN:HG2	1:A:567:PRO:HG3	1.69	0.72
1:A:232:VAL:HB	1:A:344:GLY:HA2	1.75	0.69
1:D:532:LEU:HB3	1:D:595:TYR:HB2	1.75	0.67
1:B:274:ASP:HA	1:B:277:ASN:HB2	1.77	0.66
1:C:532:LEU:HB3	1:C:595:TYR:HB2	1.77	0.66
1:D:438:CYS:SG	1:D:442:CYS:HB2	2.36	0.66
1:B:457:LEU:HB2	1:B:515:THR:HG22	1.79	0.64
1:C:440:SER:O	1:C:441:ASN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ILE:HG21	1:C:496:TRP:HB2	1.80	0.63
1:D:205:SER:HG	1:D:206:TYR:N	1.97	0.62
1:C:161:VAL:HB	1:C:164:ARG:HG3	1.81	0.62
1:D:449:LEU:HD11	1:D:457:LEU:HB3	1.83	0.61
1:B:438:CYS:CB	1:B:442:CYS:HG	2.13	0.61
1:D:578:ARG:HH21	1:D:579:LYS:HE2	1.66	0.60
1:A:80:VAL:HG11	1:A:187:TRP:CZ2	2.37	0.60
1:D:438:CYS:HG	1:D:442:CYS:HG	1.50	0.60
1:A:494:LYS:HB2	1:A:495:PRO:HD3	1.83	0.59
1:B:438:CYS:HB3	1:B:442:CYS:HG	1.67	0.59
1:D:651:HIS:HD2	1:D:656:GLU:O	1.85	0.59
1:B:438:CYS:HG	1:B:442:CYS:HG	1.48	0.59
1:A:621:PHE:CG	1:A:622:PRO:HA	2.37	0.59
1:B:438:CYS:SG	1:B:442:CYS:SG	3.01	0.58
1:C:438:CYS:HB3	1:C:442:CYS:HG	1.68	0.58
1:B:340:GLU:HB2	1:B:370:HIS:CG	2.38	0.58
1:D:112:TYR:OH	2:D:3598:PG9:OXT	2.20	0.58
1:B:440:SER:O	1:B:441:ASN:HB2	2.03	0.57
1:D:399:ARG:HB3	1:D:400:PRO:HD3	1.86	0.57
1:A:477:PRO:HB2	1:A:621:PHE:HB2	1.85	0.57
1:A:204:SER:HA	1:A:228:GLU:O	2.05	0.57
1:B:204:SER:HA	1:B:228:GLU:O	2.05	0.57
1:B:438:CYS:HB3	1:B:442:CYS:SG	2.45	0.57
1:A:111:PRO:HG3	1:A:206:TYR:CG	2.40	0.57
1:D:204:SER:HA	1:D:228:GLU:O	2.05	0.56
1:C:479:PRO:HA	1:C:621:PHE:O	2.05	0.56
1:D:274:ASP:HB2	1:D:486:ALA:HA	1.88	0.56
1:A:556:PRO:HB2	1:B:120:ARG:CZ	2.36	0.56
1:C:438:CYS:SG	1:C:439:GLU:N	2.78	0.56
1:D:574:ARG:HB3	1:D:577:TYR:HD1	1.71	0.56
1:A:576:ARG:NH1	1:A:632:VAL:O	2.34	0.56
1:A:553:ALA:HB1	1:D:271:ASP:HA	1.88	0.55
1:B:176:ASP:OD1	1:B:179:THR:HG23	2.06	0.55
1:D:232:VAL:HB	1:D:344:GLY:CA	2.33	0.55
1:C:209:PHE:HB2	1:C:231:MET:HB2	1.88	0.55
1:D:91:TYR:HE2	1:D:93:VAL:CG2	2.19	0.55
1:C:512:THR:HG23	1:C:615:GLN:HG3	1.88	0.55
1:A:274:ASP:HA	1:A:277:ASN:HB2	1.88	0.55
1:C:181:ALA:O	1:C:185:VAL:HG23	2.07	0.54
1:B:89:LYS:O	1:B:157:GLN:HG3	2.08	0.54
1:A:205:SER:OG	2:A:3600:PG9:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:HB	1:A:613:MET:HB3	1.90	0.53
1:C:204:SER:HA	1:C:228:GLU:O	2.09	0.53
1:C:438:CYS:CB	1:C:442:CYS:HG	2.21	0.53
1:D:221:ALA:O	1:D:223:LYS:HG2	2.09	0.53
1:A:232:VAL:HG11	1:A:318:ASP:HB3	1.92	0.52
1:C:438:CYS:HG	1:C:442:CYS:HG	1.57	0.52
1:D:535:ALA:HB2	1:D:592:THR:HA	1.92	0.52
1:B:535:ALA:HB2	1:B:592:THR:HA	1.92	0.52
1:B:200:GLY:HA3	1:B:406:LEU:HD11	1.91	0.51
1:B:78:ARG:HB3	1:B:94:ILE:HB	1.92	0.51
1:D:480:PHE:HE1	1:D:622:PRO:HD2	1.74	0.51
1:A:161:VAL:HB	1:A:164:ARG:HG3	1.92	0.51
1:C:88:VAL:HG13	1:C:157:GLN:HB2	1.93	0.51
1:C:373:VAL:O	1:C:394:ARG:NH1	2.43	0.51
1:D:416:PRO:HB2	1:D:431:TYR:O	2.10	0.51
1:C:457:LEU:HB2	1:C:515:THR:HG22	1.91	0.51
1:D:164:ARG:NH2	1:D:175:THR:O	2.43	0.51
1:A:340:GLU:HB2	1:A:370:HIS:CG	2.46	0.51
1:C:477:PRO:HB2	1:C:621:PHE:HB2	1.91	0.51
1:D:621:PHE:CG	1:D:622:PRO:HA	2.46	0.51
1:D:205:SER:HA	1:D:229:SER:O	2.11	0.51
1:C:229:SER:OG	1:C:338:ASP:OD1	2.29	0.51
1:C:438:CYS:HB3	1:C:442:CYS:SG	2.50	0.51
1:B:274:ASP:HB2	1:B:486:ALA:HA	1.93	0.51
1:A:481:ILE:HD11	1:A:485:PHE:CD1	2.46	0.50
1:C:621:PHE:CD1	1:C:622:PRO:HA	2.46	0.50
1:D:340:GLU:HB2	1:D:370:HIS:CG	2.46	0.50
1:A:438:CYS:HG	1:A:442:CYS:CB	2.24	0.50
1:C:404:GLU:HG3	1:C:412:SER:HA	1.93	0.50
1:A:301:ARG:HG3	1:A:301:ARG:HH11	1.76	0.50
1:B:340:GLU:OE2	2:B:3599:PG9:HA	2.11	0.50
1:B:508:PRO:HG2	1:C:508:PRO:HG2	1.94	0.50
1:D:340:GLU:OE2	2:D:3598:PG9:HA	2.12	0.50
1:B:574:ARG:HG2	1:B:576:ARG:HG2	1.94	0.50
1:C:340:GLU:HB2	1:C:370:HIS:CG	2.46	0.49
1:A:481:ILE:HG21	1:A:496:TRP:HB2	1.94	0.49
1:B:308:TYR:O	1:B:313:GLN:NE2	2.45	0.49
1:D:70:ASP:HA	1:D:73:ARG:HD3	1.94	0.49
1:B:111:PRO:HG3	1:B:206:TYR:CG	2.47	0.49
1:A:104:PRO:HB3	1:A:406:LEU:HB3	1.94	0.49
1:A:83:PRO:HA	1:A:89:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:PRO:C	1:B:630:LYS:H	2.18	0.49
1:B:457:LEU:HB2	1:B:515:THR:CG2	2.42	0.49
1:C:111:PRO:HG3	1:C:206:TYR:CG	2.48	0.49
1:A:92:THR:HG23	1:A:148:GLN:HB2	1.94	0.49
1:A:328:VAL:O	1:A:330:MET:HG3	2.13	0.49
1:C:232:VAL:HB	1:C:344:GLY:HA2	1.94	0.49
1:C:449:LEU:HD21	1:C:457:LEU:HD13	1.95	0.49
1:C:107:LEU:HD12	1:C:108:THR:N	2.28	0.49
1:C:274:ASP:HB2	1:C:486:ALA:HA	1.95	0.49
1:D:434:TRP:CG	1:D:435:PRO:HA	2.47	0.49
1:A:209:PHE:HB2	1:A:231:MET:HB2	1.94	0.48
1:D:246:PHE:O	1:D:624:TYR:HA	2.12	0.48
1:D:651:HIS:CD2	1:D:656:GLU:HB2	2.48	0.48
1:C:85:ARG:CZ	1:C:179:THR:HB	2.43	0.48
1:D:88:VAL:HG13	1:D:157:GLN:HB2	1.94	0.48
1:D:370:HIS:C	1:D:372:GLY:H	2.22	0.48
1:D:604:HIS:CG	1:D:605:VAL:H	2.32	0.48
1:B:621:PHE:CD1	1:B:622:PRO:HA	2.49	0.48
1:A:628:PRO:HA	1:A:643:TYR:CD1	2.49	0.48
1:A:91:TYR:HE2	1:A:93:VAL:CG2	2.26	0.48
1:C:416:PRO:HB2	1:C:431:TYR:O	2.14	0.48
1:A:110:THR:HB	1:A:207:GLU:HG2	1.96	0.47
1:A:532:LEU:HA	1:A:658:THR:HG23	1.96	0.47
1:A:621:PHE:CD1	1:A:622:PRO:HA	2.50	0.47
1:C:242:HIS:CD2	1:C:247:ARG:HD2	2.48	0.47
1:C:469:SER:HA	1:C:648:GLN:O	2.13	0.47
1:A:67:MET:HA	1:A:68:PRO:HD3	1.78	0.47
1:B:532:LEU:HA	1:B:658:THR:HG23	1.95	0.47
1:D:438:CYS:HG	1:D:442:CYS:CB	2.27	0.47
1:C:200:GLY:HA3	1:C:406:LEU:HD11	1.95	0.47
1:D:479:PRO:HA	1:D:621:PHE:O	2.14	0.47
1:C:81:MET:HB3	1:C:89:LYS:HB3	1.97	0.47
1:C:549:ASP:OD1	1:C:604:HIS:NE2	2.45	0.47
1:A:111:PRO:HG3	1:A:206:TYR:CD2	2.49	0.47
1:B:621:PHE:CG	1:B:622:PRO:HA	2.50	0.47
1:B:546:LYS:HB2	1:B:615:GLN:HB2	1.96	0.47
1:D:94:ILE:HG23	1:D:146:VAL:HG22	1.97	0.47
1:B:67:MET:HA	1:B:68:PRO:HD3	1.75	0.47
1:B:255:VAL:HG12	1:B:265:ASN:O	2.15	0.47
1:D:629:GLN:NE2	1:D:644:THR:O	2.41	0.47
1:A:480:PHE:CE1	1:A:622:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:PRO:HG3	1:D:206:TYR:CG	2.50	0.47
1:D:438:CYS:SG	1:D:442:CYS:CB	3.03	0.47
1:D:477:PRO:HB2	1:D:621:PHE:HB2	1.96	0.47
1:B:479:PRO:HA	1:B:621:PHE:O	2.14	0.46
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.79	0.46
1:B:62:PRO:HB2	1:B:64:SER:O	2.15	0.46
1:A:438:CYS:SG	1:A:442:CYS:HB2	2.55	0.46
1:A:507:ARG:HB3	1:A:509:ASP:OD2	2.16	0.46
1:C:67:MET:HA	1:C:68:PRO:HD3	1.84	0.46
1:D:442:CYS:O	1:D:443:THR:C	2.58	0.46
1:C:221:ALA:O	1:C:223:LYS:HG2	2.15	0.46
1:C:556:PRO:HG3	1:D:129:GLU:HA	1.97	0.46
1:B:340:GLU:HB2	1:B:370:HIS:CD2	2.51	0.46
1:C:120:ARG:CZ	1:D:556:PRO:HB2	2.46	0.46
1:D:369:ARG:H	1:D:369:ARG:HG3	1.61	0.46
1:B:416:PRO:HB2	1:B:431:TYR:O	2.14	0.46
1:B:496:TRP:HA	1:B:499:GLN:HG2	1.96	0.46
1:C:146:VAL:HG11	1:C:188:LEU:HD11	1.97	0.46
1:C:480:PHE:CE1	1:C:622:PRO:HD2	2.51	0.46
1:D:480:PHE:CE1	1:D:622:PRO:HD2	2.49	0.46
1:A:223:LYS:HE3	3:A:2433:GOL:H2	1.97	0.46
1:C:621:PHE:CG	1:C:622:PRO:HA	2.51	0.46
1:D:85:ARG:N	1:D:183:ASP:OD2	2.48	0.46
1:A:540:ASP:O	1:A:629:GLN:HA	2.16	0.46
1:B:81:MET:HB3	1:B:89:LYS:HB3	1.98	0.46
1:A:574:ARG:HB3	1:A:577:TYR:HD1	1.81	0.46
1:D:228:GLU:O	1:D:229:SER:C	2.58	0.46
1:B:205:SER:HB3	1:B:206:TYR:H	1.47	0.46
1:C:481:ILE:HD11	1:C:485:PHE:CD1	2.51	0.46
1:A:237:GLY:HA2	1:A:242:HIS:HA	1.99	0.45
1:A:274:ASP:HB2	1:A:486:ALA:HA	1.99	0.45
1:B:153:LYS:HA	1:B:153:LYS:HD2	1.66	0.45
1:C:224:VAL:HG23	1:C:329:PRO:HB2	1.97	0.45
1:C:334:GLN:HB3	1:C:345:ALA:HB3	1.99	0.45
1:A:480:PHE:HE1	1:A:622:PRO:HD2	1.82	0.45
1:C:296:TYR:O	1:C:300:GLN:HG3	2.16	0.45
1:C:552:PRO:HD3	1:C:610:HIS:CE1	2.51	0.45
1:D:70:ASP:N	1:D:70:ASP:OD1	2.49	0.45
1:D:91:TYR:CE2	1:D:93:VAL:CG2	2.99	0.45
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.69	0.45
1:C:228:GLU:O	1:C:229:SER:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:SER:HB3	1:C:647:THR:H	1.80	0.45
1:D:330:MET:HE3	1:D:330:MET:HB2	1.77	0.45
1:D:566:LEU:HD12	1:D:567:PRO:HD2	1.99	0.45
1:A:508:PRO:HG2	1:D:508:PRO:HG2	1.98	0.45
1:B:228:GLU:O	1:B:229:SER:C	2.59	0.45
1:C:73:ARG:HH11	1:C:123:ASN:HB3	1.82	0.45
1:D:478:VAL:HG22	1:D:507:ARG:HE	1.82	0.45
1:C:628:PRO:C	1:C:630:LYS:H	2.25	0.45
1:A:128:ARG:NH2	1:B:557:ASP:OD2	2.29	0.45
1:A:228:GLU:O	1:A:229:SER:C	2.59	0.45
1:B:185:VAL:O	1:B:189:VAL:HG13	2.17	0.45
1:B:544:VAL:O	1:B:616:ILE:HA	2.17	0.45
1:C:120:ARG:HB3	1:C:129:GLU:O	2.17	0.45
1:D:511:VAL:HG12	1:D:616:ILE:HB	1.99	0.45
1:B:216:LEU:HD23	1:B:321:LEU:HD12	1.99	0.44
1:B:544:VAL:HB	1:B:617:GLN:HG2	1.99	0.44
1:D:481:ILE:HG21	1:D:496:TRP:HB2	1.99	0.44
1:D:67:MET:HA	1:D:68:PRO:HD3	1.79	0.44
1:D:124:ALA:CB	1:D:129:GLU:HB3	2.48	0.44
1:A:271:ASP:HA	1:D:553:ALA:HB1	1.99	0.44
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.78	0.44
1:A:604:HIS:CG	1:A:605:VAL:H	2.35	0.44
1:B:494:LYS:HB2	1:B:495:PRO:HD3	2.00	0.44
1:B:514:GLU:HG3	1:B:611:ARG:NH2	2.33	0.44
1:D:91:TYR:HE2	1:D:93:VAL:HG23	1.83	0.44
1:A:161:VAL:O	1:A:162:MET:C	2.61	0.44
1:B:481:ILE:HG21	1:B:496:TRP:HB2	1.99	0.44
1:B:529:VAL:HG11	1:B:596:HIS:CE1	2.53	0.44
1:D:515:THR:O	1:D:611:ARG:NH2	2.51	0.44
1:A:354:ASP:C	1:A:356:ASP:H	2.24	0.44
1:C:510:VAL:HG22	1:C:617:GLN:HB3	2.00	0.44
1:A:121:VAL:HB	1:A:124:ALA:HB2	2.00	0.43
1:A:146:VAL:HG11	1:A:188:LEU:HD11	2.00	0.43
1:A:224:VAL:HG23	1:A:329:PRO:HB2	2.00	0.43
1:B:417:ASP:OD2	1:B:433:SER:HA	2.18	0.43
1:C:106:LEU:HD23	1:C:145:ARG:CZ	2.48	0.43
1:D:370:HIS:C	1:D:372:GLY:N	2.76	0.43
1:A:334:GLN:HB3	1:A:345:ALA:HB3	2.00	0.43
1:A:604:HIS:CG	1:A:605:VAL:N	2.87	0.43
1:B:164:ARG:NH2	1:B:173:THR:OG1	2.51	0.43
1:B:523:ARG:HG3	1:B:523:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:VAL:HB	1:B:661:LEU:HB2	1.99	0.43
1:C:574:ARG:HB3	1:C:577:TYR:HD1	1.82	0.43
1:C:438:CYS:SG	1:C:442:CYS:SG	3.14	0.43
1:D:205:SER:HB2	1:D:370:HIS:NE2	2.33	0.43
1:B:502:ARG:HG2	1:B:565:GLU:OE2	2.18	0.43
1:A:535:ALA:HB2	1:A:592:THR:HA	2.00	0.43
1:C:107:LEU:HG	1:C:201:MET:HE3	2.01	0.43
1:A:479:PRO:HA	1:A:621:PHE:O	2.19	0.43
1:C:95:VAL:HG12	1:C:127:MET:HE3	1.99	0.43
1:D:417:ASP:OD2	1:D:433:SER:HA	2.19	0.43
1:A:91:TYR:HB3	1:A:149:ASP:HB2	2.00	0.43
1:C:111:PRO:HB3	1:C:150:ILE:HD11	2.01	0.43
1:B:255:VAL:O	1:B:259:THR:OG1	2.32	0.43
1:B:330:MET:HE3	1:B:330:MET:HB2	1.86	0.43
1:B:406:LEU:O	1:B:408:PRO:HD3	2.19	0.43
1:D:91:TYR:CE2	1:D:93:VAL:HG23	2.53	0.43
1:D:110:THR:HB	1:D:207:GLU:HG2	2.01	0.43
1:D:117:ARG:HD2	1:D:117:ARG:HA	1.89	0.43
1:A:521:PRO:HA	1:A:606:PHE:O	2.19	0.42
1:B:480:PHE:HD2	1:B:496:TRP:CE3	2.37	0.42
1:C:318:ASP:OD2	1:C:319:LYS:N	2.52	0.42
1:C:527:VAL:HA	1:C:528:PRO:HD3	1.90	0.42
1:B:566:LEU:HD12	1:B:567:PRO:HD2	2.01	0.42
1:D:153:LYS:HD2	1:D:261:ARG:O	2.19	0.42
1:D:662:LEU:HA	1:D:663:PRO:HD3	1.82	0.42
1:A:221:ALA:O	1:A:223:LYS:HG2	2.19	0.42
1:B:511:VAL:HG11	1:B:650:ILE:HG13	2.02	0.42
1:D:205:SER:OG	2:D:3598:PG9:C	2.68	0.42
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.75	0.42
1:C:425:ASP:OD2	1:C:523:ARG:NH2	2.39	0.42
1:A:365:MET:HB2	1:A:420:ILE:HG23	2.01	0.42
1:B:558:ASP:OD1	1:B:560:LYS:HD3	2.19	0.42
1:C:232:VAL:HG13	1:C:317:LEU:HB2	2.01	0.42
1:A:540:ASP:OD2	1:A:576:ARG:NH2	2.46	0.42
1:C:549:ASP:OD2	1:C:549:ASP:C	2.63	0.42
1:D:365:MET:HE2	1:D:420:ILE:HG12	2.01	0.42
1:D:494:LYS:HB2	1:D:495:PRO:HD3	2.02	0.42
1:A:133:GLN:HG3	1:B:557:ASP:CG	2.44	0.42
1:A:153:LYS:HD2	1:A:153:LYS:HA	1.90	0.42
1:A:339:GLN:HE22	1:A:370:HIS:H	1.66	0.41
1:C:185:VAL:HG12	1:C:221:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:NH2	1:D:484:PRO:HG3	2.35	0.41
1:C:107:LEU:HD12	1:C:108:THR:H	1.85	0.41
1:C:343:TRP:CD2	1:C:347:HIS:CE1	3.08	0.41
1:C:583:LYS:HA	1:C:584:PRO:HD2	1.92	0.41
1:D:205:SER:OG	2:D:3598:PG9:OXT	2.38	0.41
1:C:153:LYS:HD2	1:C:261:ARG:O	2.21	0.41
1:A:55:VAL:HG22	1:C:170:LEU:HA	2.01	0.41
1:A:82:VAL:O	1:A:90:LEU:N	2.40	0.41
1:A:315:GLN:O	1:A:317:LEU:N	2.54	0.41
1:B:91:TYR:HB3	1:B:149:ASP:HB2	2.02	0.41
1:B:221:ALA:O	1:B:223:LYS:HG2	2.19	0.41
1:B:477:PRO:HB2	1:B:621:PHE:HB2	2.02	0.41
1:D:453:ASP:OD1	1:D:453:ASP:N	2.54	0.41
1:C:422:ASN:HB2	1:C:429:ASP:OD2	2.20	0.41
1:D:267:ILE:HA	1:D:268:PRO:HD2	1.89	0.41
1:B:401:PHE:HA	1:B:413:VAL:HG21	2.01	0.41
1:C:551:GLN:HG3	1:C:564:TYR:HB3	2.03	0.41
1:D:324:ARG:HD3	1:D:324:ARG:HA	1.50	0.41
1:D:355:ALA:O	1:D:356:ASP:C	2.64	0.41
1:D:523:ARG:HG2	1:D:605:VAL:HG22	2.01	0.41
1:A:512:THR:HG23	1:A:615:GLN:HG3	2.02	0.41
1:B:85:ARG:CZ	1:B:179:THR:HB	2.51	0.41
1:B:164:ARG:HA	1:B:165:PRO:HD3	1.88	0.41
1:C:369:ARG:H	1:C:369:ARG:HG3	1.59	0.41
1:A:434:TRP:CG	1:A:435:PRO:HA	2.55	0.41
1:B:480:PHE:HE1	1:B:622:PRO:HD2	1.85	0.41
1:B:545:VAL:HG11	1:B:660:ILE:HD11	2.03	0.41
1:C:121:VAL:HA	1:C:122:PRO:HD2	1.88	0.41
1:D:574:ARG:HB3	1:D:577:TYR:CD1	2.55	0.41
1:A:293:LEU:HD23	1:A:296:TYR:CD2	2.56	0.41
1:B:124:ALA:CB	1:B:129:GLU:HB3	2.51	0.40
1:B:209:PHE:HB2	1:B:231:MET:HB2	2.04	0.40
1:C:529:VAL:HB	1:C:661:LEU:HB2	2.03	0.40
1:D:73:ARG:HG3	1:D:125:LEU:HA	2.03	0.40
1:A:136:ASP:OD1	1:A:136:ASP:N	2.54	0.40
1:C:621:PHE:HA	1:C:622:PRO:HA	1.83	0.40
1:D:178:THR:HG23	1:D:213:MET:O	2.21	0.40
1:A:191:ASN:O	1:A:193:PRO:HD3	2.21	0.40
1:A:330:MET:HE3	1:A:330:MET:HB2	1.90	0.40
1:B:280:LYS:HE2	1:B:280:LYS:HB2	1.48	0.40
1:B:324:ARG:HA	1:B:324:ARG:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HA	1:C:53:LEU:HD23	1.88	0.40
1:B:399:ARG:HB3	1:B:400:PRO:HD3	2.04	0.40
1:B:583:LYS:HA	1:B:584:PRO:HD2	1.93	0.40
1:D:451:LEU:HA	1:D:457:LEU:HD23	2.03	0.40
1:A:162:MET:HB3	1:A:298:PHE:CD1	2.56	0.40
1:A:583:LYS:HA	1:A:584:PRO:HD2	1.93	0.40
1:B:232:VAL:HG11	1:B:318:ASP:HB3	2.04	0.40
1:D:302:MET:HE3	1:D:302:MET:HB2	1.95	0.40
1:D:331:LEU:HD23	1:D:362:THR:HB	2.04	0.40
1:D:540:ASP:OD2	1:D:576:ARG:NH1	2.52	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	615/652 (94%)	558 (91%)	53 (9%)	4 (1%)	18	49
1	B	615/652 (94%)	568 (92%)	46 (8%)	1 (0%)	43	71
1	C	615/652 (94%)	569 (92%)	41 (7%)	5 (1%)	16	45
1	D	615/652 (94%)	558 (91%)	53 (9%)	4 (1%)	18	49
All	All	2460/2608 (94%)	2253 (92%)	193 (8%)	14 (1%)	21	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	344	GLY
1	A	316	ALA
1	A	344	GLY
1	B	344	GLY
1	C	344	GLY

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Mol	Chain	Res	Type
1	C	316	ALA
1	A	237	GLY
1	C	441	ASN
1	D	345	ALA
1	D	371	SER
1	A	495	PRO
1	C	113	ASN
1	D	495	PRO
1	C	237	GLY

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	517/544 (95%)	469 (91%)	48 (9%)	8	30
1	B	517/544 (95%)	465 (90%)	52 (10%)	7	26
1	C	517/544 (95%)	458 (89%)	59 (11%)	5	21
1	D	517/544 (95%)	460 (89%)	57 (11%)	6	23
All	All	2068/2176 (95%)	1852 (90%)	216 (10%)	7	25

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	56	GLN
1	A	64	SER
1	A	65	VAL
1	A	67	MET
1	A	71	GLN
1	A	77	LYS
1	A	107	LEU
1	A	110	THR
1	A	120	ARG
1	A	130	VAL
1	A	195	SER

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Mol	Chain	Res	Type
1	A	198	ARG
1	A	201	MET
1	A	205	SER
1	A	229	SER
1	A	239	ASP
1	A	256	SER
1	A	258	MET
1	A	280	LYS
1	A	290	GLN
1	A	319	LYS
1	A	339	GLN
1	A	346	ILE
1	A	399	ARG
1	A	427	LYS
1	A	432	ARG
1	A	440	SER
1	A	442	CYS
1	A	447	THR
1	A	453	ASP
1	A	471	VAL
1	A	472	SER
1	A	490	SER
1	A	491	SER
1	A	503	GLU
1	A	511	VAL
1	A	523	ARG
1	A	524	VAL
1	A	536	THR
1	A	539	THR
1	A	541	SER
1	A	615	GLN
1	A	620	TRP
1	A	629	GLN
1	A	630	LYS
1	A	632	VAL
1	A	644	THR
1	B	57	THR
1	B	64	SER
1	B	65	VAL
1	B	67	MET
1	B	80	VAL
1	B	94	ILE

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Mol	Chain	Res	Type
1	B	98	LYS
1	B	99	ASN
1	B	107	LEU
1	B	120	ARG
1	B	126	THR
1	B	157	GLN
1	B	189	VAL
1	B	201	MET
1	B	205	SER
1	B	223	LYS
1	B	242	HIS
1	B	256	SER
1	B	276	THR
1	B	279	LEU
1	B	280	LYS
1	B	313	GLN
1	B	319	LYS
1	B	325	LYS
1	B	331	LEU
1	B	379	THR
1	B	392	GLN
1	B	395	ARG
1	B	412	SER
1	B	415	LEU
1	B	425	ASP
1	B	427	LYS
1	B	438	CYS
1	B	443	THR
1	B	469	SER
1	B	472	SER
1	B	482	SER
1	B	516	GLU
1	B	519	ASP
1	B	520	GLU
1	B	523	ARG
1	B	532	LEU
1	B	539	THR
1	B	560	LYS
1	B	565	GLU
1	B	598	THR
1	B	620	TRP
1	B	629	GLN

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Mol	Chain	Res	Type
1	B	648	GLN
1	B	649	SER
1	B	665	VAL
1	B	666	LYS
1	C	54	SER
1	C	57	THR
1	C	65	VAL
1	C	66	HIS
1	C	71	GLN
1	C	72	GLN
1	C	77	LYS
1	C	80	VAL
1	C	85	ARG
1	C	98	LYS
1	C	120	ARG
1	C	123	ASN
1	C	126	THR
1	C	129	GLU
1	C	130	VAL
1	C	140	GLU
1	C	144	ILE
1	C	174	LYS
1	C	175	THR
1	C	201	MET
1	C	205	SER
1	C	209	PHE
1	C	222	LEU
1	C	270	ARG
1	C	280	LYS
1	C	325	LYS
1	C	330	MET
1	C	331	LEU
1	C	346	ILE
1	C	357	VAL
1	C	379	THR
1	C	392	GLN
1	C	395	ARG
1	C	427	LYS
1	C	432	ARG
1	C	438	CYS
1	C	453	ASP
1	C	465	ASP

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Mol	Chain	Res	Type
1	C	482	SER
1	C	490	SER
1	C	491	SER
1	C	494	LYS
1	C	506	SER
1	C	518	LEU
1	C	523	ARG
1	C	537	SER
1	C	546	LYS
1	C	560	LYS
1	C	576	ARG
1	C	583	LYS
1	C	615	GLN
1	C	616	ILE
1	C	620	TRP
1	C	621	PHE
1	C	629	GLN
1	C	644	THR
1	C	648	GLN
1	C	649	SER
1	C	655	LYS
1	D	61	ILE
1	D	64	SER
1	D	65	VAL
1	D	69	THR
1	D	70	ASP
1	D	71	GLN
1	D	72	GLN
1	D	73	ARG
1	D	80	VAL
1	D	101	ARG
1	D	115	LYS
1	D	120	ARG
1	D	126	THR
1	D	130	VAL
1	D	204	SER
1	D	205	SER
1	D	215	LEU
1	D	265	ASN
1	D	276	THR
1	D	280	LYS
1	D	293	LEU

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Mol	Chain	Res	Type
1	D	324	ARG
1	D	325	LYS
1	D	327	THR
1	D	331	LEU
1	D	358	LYS
1	D	365	MET
1	D	379	THR
1	D	395	ARG
1	D	407	LYS
1	D	417	ASP
1	D	436	SER
1	D	440	SER
1	D	442	CYS
1	D	447	THR
1	D	449	LEU
1	D	460	THR
1	D	472	SER
1	D	482	SER
1	D	491	SER
1	D	506	SER
1	D	516	GLU
1	D	518	LEU
1	D	539	THR
1	D	541	SER
1	D	611	ARG
1	D	616	ILE
1	D	620	TRP
1	D	626	ARG
1	D	630	LYS
1	D	635	ILE
1	D	639	LYS
1	D	644	THR
1	D	647	THR
1	D	649	SER
1	D	655	LYS
1	D	665	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	167	HIS
1	A	191	ASN
1	A	248	GLN
1	A	295	GLN
1	A	339	GLN
1	A	441	ASN
1	B	71	GLN
1	B	72	GLN
1	B	123	ASN
1	B	133	GLN
1	B	167	HIS
1	B	300	GLN
1	B	313	GLN
1	B	361	ASN
1	B	392	GLN
1	B	455	HIS
1	B	629	GLN
1	B	648	GLN
1	B	651	HIS
1	C	167	HIS
1	C	441	ASN
1	D	133	GLN
1	D	167	HIS
1	D	455	HIS
1	D	594	HIS
1	D	617	GLN
1	D	651	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

7 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	GOL	A	2433	-	5,5,5	0.42	0	5,5,5	0.23	0
2	PG9	B	3599	-	10,11,11	1.82	1 (10%)	8,14,14	1.05	1 (12%)
3	GOL	C	2430	-	5,5,5	0.42	0	5,5,5	0.15	0
3	GOL	A	2431	-	5,5,5	0.34	0	5,5,5	0.33	0
3	GOL	B	2432	-	5,5,5	0.31	0	5,5,5	0.31	0
2	PG9	A	3600	-	10,11,11	1.54	1 (10%)	8,14,14	1.12	1 (12%)
2	PG9	D	3598	-	10,11,11	1.70	2 (20%)	8,14,14	1.08	1 (12%)

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	A	2433	-	-	2/4/4/4	-
2	PG9	B	3599	-	-	1/8/8/8	0/1/1/1
3	GOL	C	2430	-	-	2/4/4/4	-
3	GOL	A	2431	-	-	1/4/4/4	-
3	GOL	B	2432	-	-	0/4/4/4	-
2	PG9	A	3600	-	-	2/8/8/8	0/1/1/1
2	PG9	D	3598	-	-	2/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3599	PG9	CB-CA	-4.97	1.47	1.52
2	D	3598	PG9	CB-CA	-4.49	1.47	1.52
2	A	3600	PG9	CB-CA	-3.91	1.48	1.52
2	D	3598	PG9	OXT-C	-2.01	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3600	PG9	OXT-C-O	-2.13	119.26	124.08
2	D	3598	PG9	OXT-C-O	-2.08	119.36	124.08
2	B	3599	PG9	CG2-CB-CG1	2.03	120.82	118.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3600	PG9	O-C-CA-N
3	A	2433	GOL	O1-C1-C2-C3
3	C	2430	GOL	O1-C1-C2-C3
3	A	2433	GOL	O1-C1-C2-O2
3	A	2431	GOL	C1-C2-C3-O3
3	C	2430	GOL	O1-C1-C2-O2
2	B	3599	PG9	O-C-CA-N
2	D	3598	PG9	O-C-CA-N
2	D	3598	PG9	OXT-C-CA-N
2	A	3600	PG9	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2433	GOL	1	0
2	B	3599	PG9	1	0
2	A	3600	PG9	1	0
2	D	3598	PG9	4	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	617/652 (94%)	-0.13	12 (1%) 66 48	19, 19, 19, 19	0
1	B	617/652 (94%)	-0.12	12 (1%) 66 48	19, 19, 19, 19	0
1	C	617/652 (94%)	-0.09	18 (2%) 53 35	19, 19, 19, 19	0
1	D	617/652 (94%)	-0.08	11 (1%) 67 49	19, 19, 19, 19	0
All	All	2468/2608 (94%)	-0.11	53 (2%) 63 44	19, 19, 19, 19	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ASP	8.0
1	D	69	THR	6.3
1	B	69	THR	6.2
1	C	70	ASP	5.8
1	A	70	ASP	5.6
1	D	70	ASP	5.6
1	A	69	THR	5.5
1	A	66	HIS	5.0
1	B	99	ASN	4.8
1	A	50	HIS	4.4
1	B	50	HIS	4.2
1	C	66	HIS	4.1
1	D	66	HIS	4.1
1	A	68	PRO	3.9
1	D	50	HIS	3.9
1	C	101	ARG	3.8
1	C	69	THR	3.8
1	B	66	HIS	3.7
1	C	72	GLN	3.7
1	C	67	MET	3.7
1	D	71	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	67	MET	3.4
1	A	519	ASP	3.4
1	D	67	MET	3.4
1	C	50	HIS	3.1
1	C	68	PRO	3.0
1	C	71	GLN	3.0
1	A	265	ASN	3.0
1	B	453	ASP	2.8
1	A	666	LYS	2.8
1	D	99	ASN	2.7
1	C	265	ASN	2.7
1	A	72	GLN	2.7
1	D	101	ARG	2.7
1	B	71	GLN	2.6
1	B	441	ASN	2.6
1	D	63	ALA	2.6
1	D	453	ASP	2.6
1	A	516	GLU	2.4
1	C	65	VAL	2.4
1	B	63	ALA	2.3
1	A	295	GLN	2.3
1	B	67	MET	2.3
1	B	68	PRO	2.3
1	D	68	PRO	2.2
1	C	653	GLY	2.2
1	C	441	ASN	2.2
1	C	64	SER	2.1
1	C	264	GLY	2.1
1	C	295	GLN	2.1
1	C	63	ALA	2.1
1	B	356	ASP	2.0
1	C	519	ASP	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($\text{\AA}^2$)	Q<0.9
3	GOL	A	2431	6/6	0.70	0.17	19,19,19,19	0
3	GOL	C	2430	6/6	0.75	0.20	19,19,19,19	0
3	GOL	A	2433	6/6	0.81	0.15	19,19,19,19	0
2	PG9	A	3600	11/11	0.90	0.23	19,19,19,19	0
3	GOL	B	2432	6/6	0.91	0.14	19,19,19,19	0
2	PG9	D	3598	11/11	0.92	0.17	19,19,19,19	0
2	PG9	B	3599	11/11	0.93	0.22	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.