



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:28 PM GMT

PDB ID : 3S9M
Title : Complex between transferrin receptor 1 and transferrin with iron in the N-Lobe, cryocooled 1
Authors : Eckenroth, B.E.; Steere, A.N.; Mason, A.B.; Everse, S.J.
Deposited on : 2011-06-01
Resolution : 3.32 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

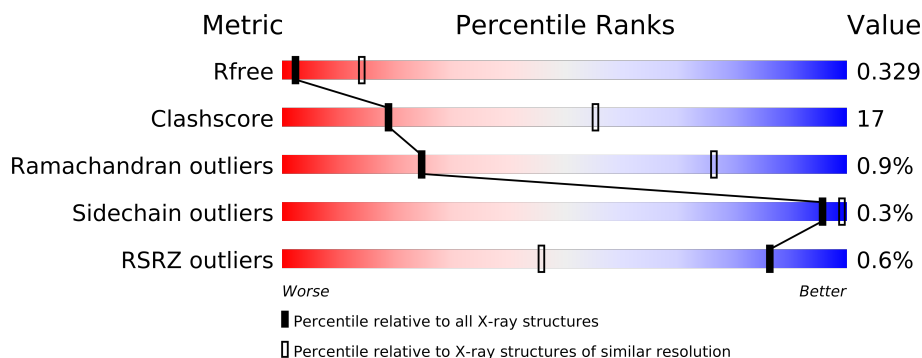
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1372 (3.44-3.20)
Clashscore	79885	1016 (3.42-3.22)
Ramachandran outliers	78287	1699 (3.44-3.20)
Sidechain outliers	78261	1697 (3.44-3.20)
RSRZ outliers	66119	1373 (3.44-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	654	
1	B	654	
2	C	693	
2	D	693	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	903	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16658 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4917	3149	820	934	14			
1	B	639	Total	C	N	O	S	0	0	0
			4773	3056	790	913	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	VAL	-	EXPRESSION TAG	UNP P02786
A	108	PRO	-	EXPRESSION TAG	UNP P02786
A	109	ASP	-	EXPRESSION TAG	UNP P02786
A	110	LYS	-	EXPRESSION TAG	UNP P02786
A	111	HIS	-	EXPRESSION TAG	UNP P02786
A	112	HIS	-	EXPRESSION TAG	UNP P02786
A	113	HIS	-	EXPRESSION TAG	UNP P02786
A	114	HIS	-	EXPRESSION TAG	UNP P02786
A	115	HIS	-	EXPRESSION TAG	UNP P02786
A	116	HIS	-	EXPRESSION TAG	UNP P02786
A	117	ILE	-	EXPRESSION TAG	UNP P02786
A	118	GLU	-	EXPRESSION TAG	UNP P02786
A	119	GLY	-	EXPRESSION TAG	UNP P02786
A	142	SER	GLY	SEE REMARK 999	UNP P02786
B	107	VAL	-	EXPRESSION TAG	UNP P02786
B	108	PRO	-	EXPRESSION TAG	UNP P02786
B	109	ASP	-	EXPRESSION TAG	UNP P02786
B	110	LYS	-	EXPRESSION TAG	UNP P02786
B	111	HIS	-	EXPRESSION TAG	UNP P02786
B	112	HIS	-	EXPRESSION TAG	UNP P02786
B	113	HIS	-	EXPRESSION TAG	UNP P02786
B	114	HIS	-	EXPRESSION TAG	UNP P02786
B	115	HIS	-	EXPRESSION TAG	UNP P02786
B	116	HIS	-	EXPRESSION TAG	UNP P02786
B	117	ILE	-	EXPRESSION TAG	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLU	-	EXPRESSION TAG	UNP P02786
B	119	GLY	-	EXPRESSION TAG	UNP P02786
B	142	SER	GLY	SEE REMARK 999	UNP P02786

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	517	Total	C	N	O	S	0	0	0
			3682	2305	623	718	36			
2	D	488	Total	C	N	O	S	0	0	0
			3246	1988	565	662	31			

There are 38 discrepancies between the modelled and reference sequences:

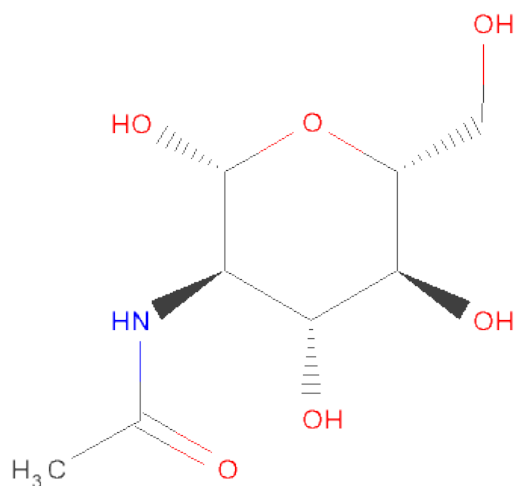
Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	VAL	-	EXPRESSION TAG	UNP P02787
C	-12	PRO	-	EXPRESSION TAG	UNP P02787
C	-11	ASP	-	EXPRESSION TAG	UNP P02787
C	-10	LYS	-	EXPRESSION TAG	UNP P02787
C	-9	HIS	-	EXPRESSION TAG	UNP P02787
C	-8	HIS	-	EXPRESSION TAG	UNP P02787
C	-7	HIS	-	EXPRESSION TAG	UNP P02787
C	-6	HIS	-	EXPRESSION TAG	UNP P02787
C	-5	HIS	-	EXPRESSION TAG	UNP P02787
C	-4	HIS	-	EXPRESSION TAG	UNP P02787
C	-3	ILE	-	EXPRESSION TAG	UNP P02787
C	-2	GLU	-	EXPRESSION TAG	UNP P02787
C	-1	GLY	-	EXPRESSION TAG	UNP P02787
C	0	ARG	-	EXPRESSION TAG	UNP P02787
C	413	ASP	ASN	ENGINEERED MUTATION	UNP P02787
C	426	PHE	TYR	ENGINEERED MUTATION	UNP P02787
C	429	VAL	ILE	SEE REMARK 999	UNP P02787
C	517	PHE	TYR	ENGINEERED MUTATION	UNP P02787
C	611	ASP	ASN	ENGINEERED MUTATION	UNP P02787
D	-13	VAL	-	EXPRESSION TAG	UNP P02787
D	-12	PRO	-	EXPRESSION TAG	UNP P02787
D	-11	ASP	-	EXPRESSION TAG	UNP P02787
D	-10	LYS	-	EXPRESSION TAG	UNP P02787
D	-9	HIS	-	EXPRESSION TAG	UNP P02787
D	-8	HIS	-	EXPRESSION TAG	UNP P02787
D	-7	HIS	-	EXPRESSION TAG	UNP P02787
D	-6	HIS	-	EXPRESSION TAG	UNP P02787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP P02787
D	-4	HIS	-	EXPRESSION TAG	UNP P02787
D	-3	ILE	-	EXPRESSION TAG	UNP P02787
D	-2	GLU	-	EXPRESSION TAG	UNP P02787
D	-1	GLY	-	EXPRESSION TAG	UNP P02787
D	0	ARG	-	EXPRESSION TAG	UNP P02787
D	413	ASP	ASN	ENGINEERED MUTATION	UNP P02787
D	426	PHE	TYR	ENGINEERED MUTATION	UNP P02787
D	429	VAL	ILE	SEE REMARK 999	UNP P02787
D	517	PHE	TYR	ENGINEERED MUTATION	UNP P02787
D	611	ASP	ASN	ENGINEERED MUTATION	UNP P02787

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

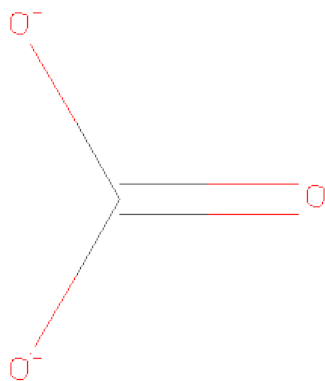
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

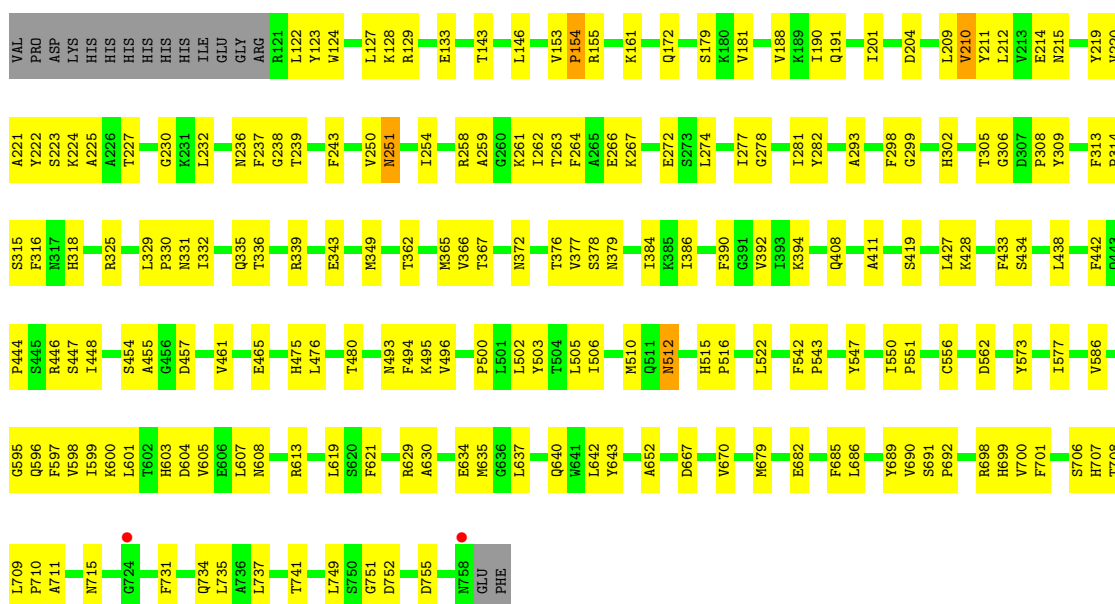
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Fe	0	0
			1	1		
6	C	1	Total	Fe	0	0
			1	1		

3 Residue-property plots

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

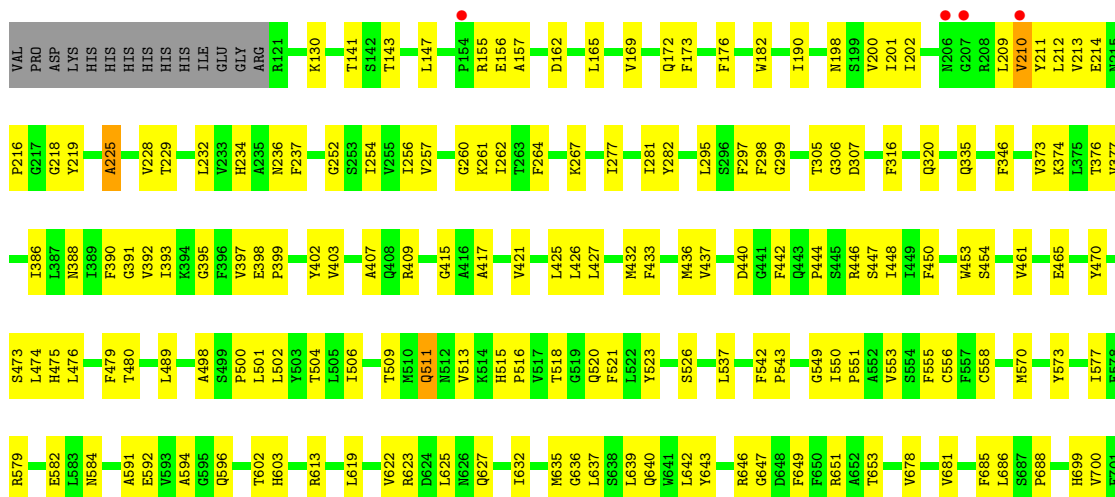
• Molecule 1: Transferrin receptor protein 1

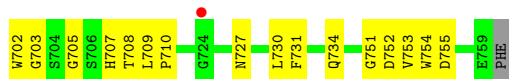
Chain A:



• Molecule 1: Transferrin receptor protein 1

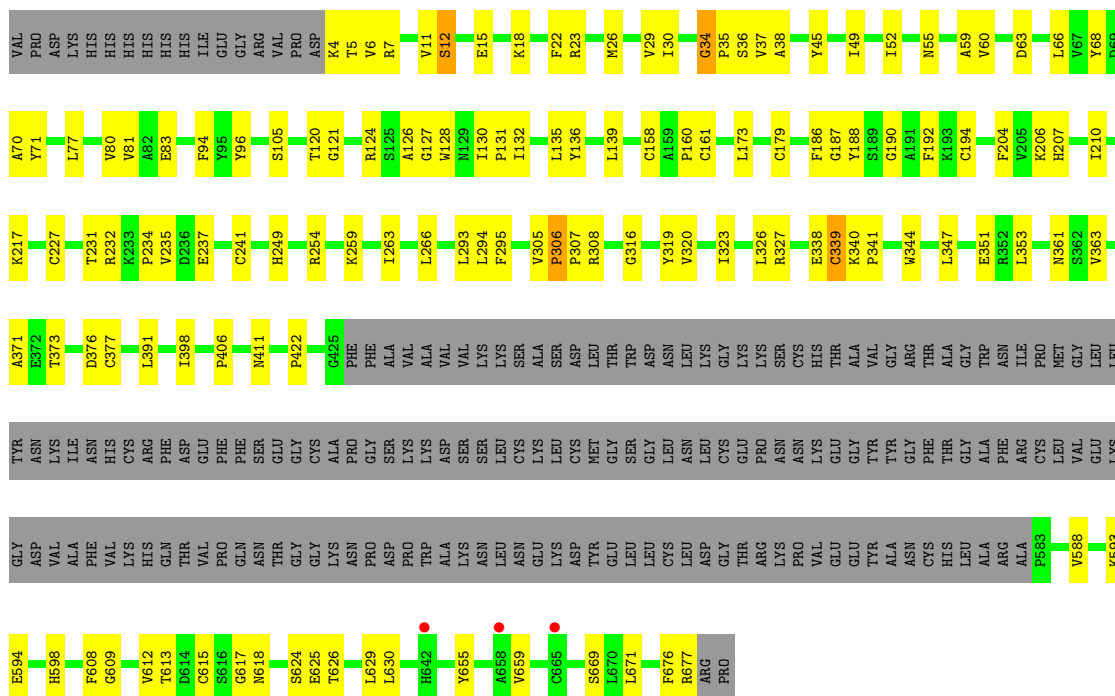
Chain B:





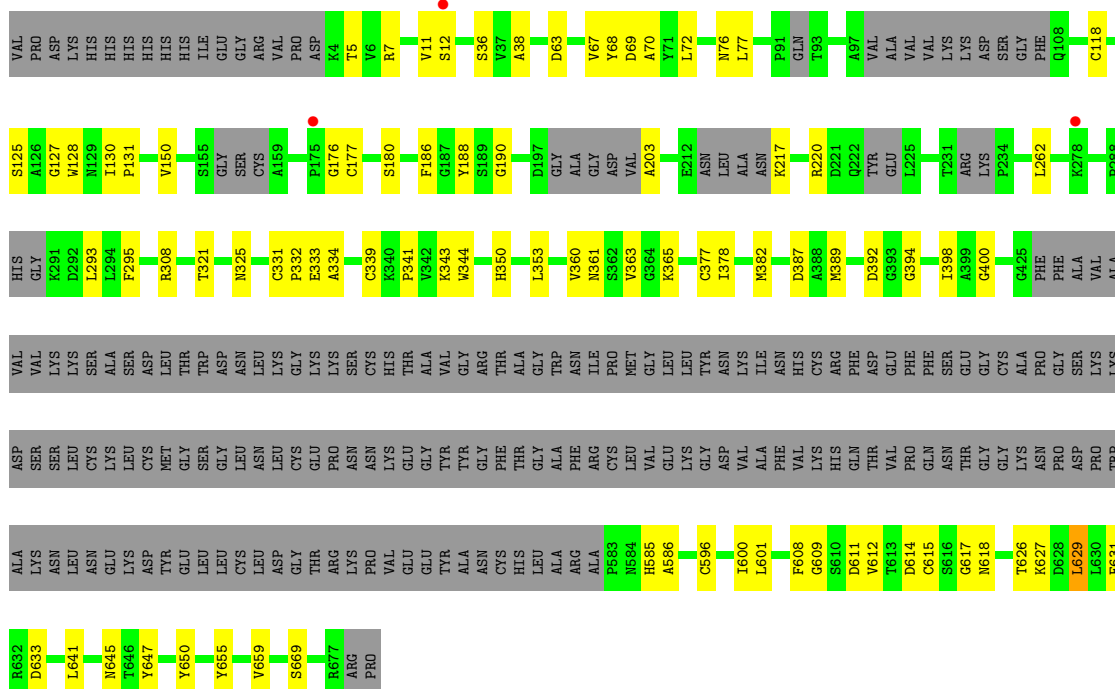
• Molecule 2: Serotransferrin

Chain C:



• Molecule 2: Serotransferrin

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	232.19Å 232.19Å 168.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 3.32 16.98 – 3.32	Depositor EDS
% Data completeness (in resolution range)	96.6 (17.00-3.32) 96.8 (16.98-3.32)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.332 0.281 , 0.329	Depositor DCC
R_{free} test set	6560 reflections (11.16%)	DCC
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 18.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 65342 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16658	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, FE, CA, NAG

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	0.43	0/5036	0.63	0/6862
1	B	0.42	0/4891	0.60	2/6688 (0.0%)
2	C	0.38	0/3760	0.58	0/5134
2	D	0.32	0/3296	0.53	0/4507
All	All	0.39	0/16983	0.59	2/23191 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	PHE	O-C-N	-7.63	110.49	122.70
1	B	316	PHE	CA-C-N	5.83	130.03	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4917	0	4680	193	0
1	B	4773	0	4386	158	0
2	C	3682	0	3265	117	0
2	D	3246	0	2625	63	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	4	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16658	0	14982	525	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (525) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:751:GLY:O	1:A:755:ASP:HB2	1.33	1.29
1:B:489:LEU:HD12	1:B:558:CYS:SG	1.75	1.26
1:A:155:ARG:O	1:A:411:ALA:O	1.57	1.19
1:B:210:VAL:HG12	1:B:211:TYR:N	1.58	1.17
1:A:210:VAL:HG12	1:A:211:TYR:H	1.01	1.10
1:A:210:VAL:HG12	1:A:211:TYR:N	1.67	1.09
1:B:210:VAL:HG12	1:B:211:TYR:H	0.92	1.08
1:A:223:SER:HB3	1:A:379:ASN:HD22	1.21	1.06
1:A:629:ARG:NH2	2:C:618:ASN:OD1	1.96	0.98
1:B:210:VAL:CG1	1:B:211:TYR:H	1.72	0.97
1:B:727:ASN:HD22	1:B:730:LEU:HB2	1.29	0.97
2:C:5:THR:HG22	2:C:36:SER:HB3	1.44	0.94
2:D:188:TYR:OH	5:D:905:CO3:O2	1.85	0.94
1:A:123:TYR:O	1:A:127:LEU:HD13	1.69	0.93
2:C:351:GLU:HG2	2:C:629:LEU:O	1.68	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:VAL:CB	1:A:154:PRO:HD3	1.99	0.93
2:C:5:THR:HG22	2:C:36:SER:CB	2.00	0.92
1:A:751:GLY:O	1:A:755:ASP:CB	2.18	0.91
1:A:210:VAL:CG1	1:A:211:TYR:H	1.82	0.91
1:B:511:GLN:O	1:B:521:PHE:CD1	2.23	0.91
1:A:599:ILE:O	1:A:603:HIS:HB2	1.72	0.90
1:B:751:GLY:O	1:B:755:ASP:HB2	1.71	0.89
2:C:26:MET:O	2:C:30:ILE:HB	1.72	0.89
2:C:227:CYS:HB2	2:C:231:THR:HG22	1.53	0.89
1:A:259:ALA:HA	1:A:267:LYS:HE3	1.53	0.89
1:A:225:ALA:HB1	1:A:378:SER:HA	1.56	0.88
1:A:222:TYR:CD2	1:A:302:HIS:HB2	2.09	0.87
1:B:256:ILE:HD11	1:B:282:TYR:CD2	2.11	0.85
1:B:264:PHE:CD2	1:B:299:GLY:HA3	2.11	0.85
2:C:340:LYS:HD2	2:C:341:PRO:HD2	1.60	0.83
1:A:204:ASP:HB2	1:A:209:LEU:CB	2.08	0.83
1:B:201:ILE:HG22	1:B:212:LEU:HA	1.62	0.82
1:B:489:LEU:CD1	1:B:558:CYS:SG	2.64	0.81
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.15	0.81
2:C:105:SER:HB2	2:C:232:ARG:HH22	1.45	0.80
1:A:277:ILE:O	1:A:332:ILE:HG23	1.81	0.79
1:A:599:ILE:O	1:A:603:HIS:CB	2.31	0.79
1:A:446:ARG:NE	1:A:607:LEU:HD21	1.98	0.79
1:B:264:PHE:HD2	1:B:299:GLY:HA3	1.48	0.78
1:B:182:TRP:HZ3	1:B:392:VAL:HG12	1.48	0.78
1:A:223:SER:HB3	1:A:379:ASN:ND2	1.97	0.78
1:A:263:THR:OG1	1:A:266:GLU:HG3	1.85	0.78
1:B:500:PRO:HB3	1:B:613:ARG:HG3	1.66	0.77
1:B:407:ALA:HB3	1:B:426:LEU:HD22	1.64	0.77
1:A:225:ALA:CA	1:A:377:VAL:O	2.33	0.77
1:A:278:GLY:HA2	1:A:332:ILE:CG2	2.15	0.76
1:B:256:ILE:HD11	1:B:282:TYR:HD2	1.48	0.76
1:A:640:GLN:HA	1:A:643:TYR:HD1	1.50	0.76
1:A:494:PHE:CE2	1:A:510:MET:SD	2.79	0.76
2:C:49:ILE:HG23	2:C:77:LEU:HD12	1.68	0.76
1:B:257:VAL:HG23	1:B:281:ILE:HG12	1.66	0.76
1:B:509:THR:HG23	1:B:596:GLN:HE21	1.51	0.75
1:B:474:LEU:HD13	1:B:550:ILE:HD11	1.66	0.75
1:A:225:ALA:HA	1:A:377:VAL:O	1.86	0.75
1:B:210:VAL:CG1	1:B:211:TYR:N	2.34	0.74
1:A:224:LYS:CB	1:A:331:ASN:O	2.35	0.74
1:A:222:TYR:CE1	1:A:308:PRO:HG3	2.22	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:227:CYS:HB2	2:C:231:THR:CG2	2.17	0.74
1:A:751:GLY:C	1:A:755:ASP:HB2	2.07	0.74
1:B:397:VAL:HG12	1:B:398:GLU:HG3	1.70	0.73
1:B:632:ILE:HG13	1:B:639:LEU:HD13	1.71	0.73
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.69	0.73
1:A:201:ILE:HG22	1:A:212:LEU:HA	1.70	0.73
2:C:29:VAL:HG23	2:C:30:ILE:HD12	1.71	0.72
1:A:225:ALA:C	1:A:377:VAL:O	2.27	0.72
1:A:494:PHE:CD2	1:A:510:MET:HE1	2.25	0.71
1:B:172:GLN:HG3	1:B:176:PHE:CE2	2.26	0.71
1:B:518:THR:OG1	1:B:520:GLN:HG2	1.89	0.70
1:B:727:ASN:ND2	1:B:730:LEU:HB2	2.04	0.70
2:D:69:ASP:HA	2:D:72:LEU:HD12	1.74	0.69
2:C:34:GLY:H	2:C:35:PRO:CD	2.04	0.69
2:D:188:TYR:OH	5:D:905:CO3:C	2.40	0.69
1:B:549:GLY:HA3	1:B:686:LEU:HD11	1.74	0.69
2:D:353:LEU:HD23	2:D:353:LEU:O	1.93	0.69
1:A:494:PHE:CD2	1:A:510:MET:CE	2.76	0.69
2:C:59:ALA:HB2	2:C:263:ILE:HD13	1.74	0.69
1:A:123:TYR:O	1:A:127:LEU:CD1	2.40	0.68
2:C:45:TYR:CE2	2:C:66:LEU:HD22	2.29	0.68
1:A:223:SER:CB	1:A:379:ASN:HD22	2.03	0.68
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.75	0.68
1:A:237:PHE:CD2	1:A:261:LYS:CB	2.77	0.68
2:D:626:THR:OG1	2:D:629:LEU:HG	1.94	0.68
1:B:442:PHE:CE2	1:B:444:PRO:HG3	2.29	0.67
1:A:512:ASN:C	1:A:512:ASN:HD22	1.95	0.67
1:A:433:PHE:HE1	1:A:599:ILE:HD11	1.60	0.67
1:A:551:PRO:CD	1:A:682:GLU:HG2	2.23	0.67
1:A:179:SER:OG	1:A:392:VAL:O	2.14	0.66
1:B:500:PRO:HB3	1:B:613:ARG:CG	2.25	0.66
2:C:319:TYR:O	2:C:323:ILE:HG13	1.96	0.66
1:B:444:PRO:HB3	1:B:602:THR:HG21	1.78	0.66
1:B:172:GLN:HG3	1:B:176:PHE:CZ	2.31	0.65
1:A:293:ALA:HB2	1:A:339:ARG:NH2	2.11	0.65
2:C:340:LYS:HD2	2:C:341:PRO:CD	2.25	0.65
1:A:298:PHE:HE2	1:A:457:ASP:HB3	1.62	0.65
2:D:641:LEU:HD13	2:D:645:ASN:HB2	1.78	0.65
1:B:257:VAL:CG2	1:B:281:ILE:HG12	2.26	0.65
2:C:340:LYS:HB3	2:C:593:LYS:HZ2	1.62	0.65
2:D:188:TYR:CZ	5:D:905:CO3:O2	2.50	0.64
2:C:217:LYS:O	2:C:217:LYS:HD3	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:PRO:HB3	1:A:613:ARG:HG3	1.80	0.64
2:C:615:CYS:O	2:C:618:ASN:O	2.15	0.64
1:B:200:VAL:HG13	1:B:213:VAL:HB	1.80	0.64
2:C:52:ILE:O	2:C:254:ARG:HD3	1.97	0.64
1:A:366:VAL:HG12	1:A:367:THR:N	2.13	0.63
2:C:45:TYR:CZ	2:C:66:LEU:HD22	2.33	0.63
2:D:615:CYS:HA	2:D:618:ASN:O	1.98	0.63
1:B:395:GLY:O	1:B:399:PRO:HG3	1.98	0.62
1:A:210:VAL:CG1	1:A:211:TYR:N	2.43	0.62
1:A:597:PHE:O	1:A:601:LEU:HG	2.00	0.62
2:C:391:LEU:HD12	2:C:588:VAL:HG21	1.81	0.62
2:C:26:MET:SD	2:C:30:ILE:HD13	2.39	0.62
2:C:340:LYS:CG	2:C:593:LYS:HZ2	2.13	0.62
2:C:49:ILE:HG23	2:C:77:LEU:CD1	2.28	0.62
2:D:344:TRP:HZ3	2:D:601:LEU:HD21	1.65	0.62
1:B:386:ILE:HG23	1:B:454:SER:HB3	1.81	0.61
2:C:340:LYS:HG2	2:C:593:LYS:NZ	2.15	0.61
1:A:272:GLU:HG3	1:A:332:ILE:CD1	2.30	0.61
1:A:129:ARG:O	1:A:133:GLU:HG3	2.00	0.61
1:B:157:ALA:HA	1:B:162:ASP:OD1	1.99	0.61
2:D:614:ASP:O	2:D:617:GLY:N	2.33	0.61
1:A:123:TYR:C	1:A:127:LEU:HD13	2.21	0.61
1:B:256:ILE:CD1	1:B:282:TYR:CD2	2.83	0.61
1:A:146:LEU:HD23	1:A:146:LEU:O	2.00	0.61
1:A:700:VAL:HG11	1:A:741:THR:HG21	1.81	0.61
1:B:475:HIS:ND1	1:B:476:LEU:HG	2.16	0.61
2:C:130:ILE:N	2:C:131:PRO:HD2	2.16	0.61
1:A:221:ALA:O	1:A:222:TYR:HB2	2.00	0.60
1:A:172:GLN:HG2	1:A:427:LEU:HD22	1.83	0.60
2:C:120:THR:OG1	2:C:127:GLY:HA3	2.01	0.60
2:D:118:CYS:HB2	2:D:203:ALA:N	2.16	0.60
1:B:165:LEU:O	1:B:169:VAL:HG23	2.02	0.60
2:C:5:THR:CG2	2:C:36:SER:HB3	2.27	0.60
1:A:446:ARG:CZ	1:A:607:LEU:HD21	2.31	0.60
1:A:127:LEU:HD23	1:A:599:ILE:HG23	1.83	0.60
1:A:220:VAL:O	1:A:223:SER:HB2	2.02	0.60
2:C:624:SER:HB3	2:C:629:LEU:HD13	1.84	0.59
1:B:256:ILE:CD1	1:B:282:TYR:HD2	2.15	0.59
2:C:340:LYS:CB	2:C:593:LYS:HZ2	2.14	0.59
2:C:338:GLU:O	2:C:339:CYS:HB2	2.02	0.59
1:B:474:LEU:CD1	1:B:550:ILE:HD11	2.31	0.59
1:B:705:GLY:HA3	1:B:707:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:7:ARG:HA	2:C:38:ALA:HB3	1.82	0.59
2:C:615:CYS:HA	2:C:618:ASN:O	2.02	0.59
2:D:5:THR:HA	2:D:36:SER:HB3	1.84	0.59
1:A:685:PHE:O	1:A:700:VAL:HG22	2.02	0.59
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.85	0.59
1:A:225:ALA:HA	1:A:377:VAL:C	2.22	0.59
1:A:446:ARG:CZ	1:A:607:LEU:CD2	2.81	0.59
1:A:551:PRO:HD3	1:A:682:GLU:HG2	1.83	0.59
2:C:351:GLU:CG	2:C:629:LEU:O	2.45	0.58
2:C:398:ILE:HG23	2:C:671:LEU:HD23	1.85	0.58
1:A:689:TYR:CD2	1:A:737:LEU:HD22	2.39	0.58
1:A:313:PHE:HB2	1:A:314:PRO:HD2	1.86	0.58
1:B:282:TYR:HH	1:B:346:PHE:HZ	1.50	0.58
2:C:135:LEU:O	2:C:139:LEU:HG	2.03	0.58
1:B:635:MET:O	1:B:637:LEU:N	2.34	0.58
1:A:264:PHE:HD1	1:A:281:ILE:HD13	1.69	0.58
2:D:70:ALA:HB1	2:D:77:LEU:HB2	1.86	0.58
1:A:506:ILE:O	1:A:510:MET:HG2	2.03	0.57
2:C:136:TYR:HA	2:C:139:LEU:HD12	1.85	0.57
2:C:34:GLY:H	2:C:35:PRO:HD2	1.69	0.57
1:A:237:PHE:CG	1:A:261:LYS:CB	2.87	0.57
2:C:23:ARG:HD3	2:C:37:VAL:O	2.03	0.57
1:A:629:ARG:NE	2:C:617:GLY:O	2.26	0.57
1:A:682:GLU:HA	1:A:682:GLU:OE1	2.03	0.57
2:C:234:PRO:HD2	2:C:237:GLU:OE1	2.04	0.57
1:B:225:ALA:HA	1:B:377:VAL:HB	1.87	0.57
1:B:172:GLN:HG2	1:B:427:LEU:HD22	1.85	0.57
2:D:615:CYS:O	2:D:618:ASN:O	2.22	0.57
1:A:433:PHE:HE1	1:A:599:ILE:CD1	2.18	0.57
2:D:130:ILE:N	2:D:131:PRO:HD2	2.19	0.57
2:C:340:LYS:HG2	2:C:593:LYS:HZ2	1.69	0.56
1:A:343:GLU:HG2	1:A:362:THR:HG21	1.86	0.56
1:A:454:SER:O	1:A:455:ALA:HB3	2.05	0.56
1:B:228:VAL:HB	1:B:277:ILE:HG22	1.86	0.56
1:A:153:VAL:CB	1:A:154:PRO:CD	2.80	0.56
1:A:222:TYR:CD2	1:A:302:HIS:CB	2.86	0.56
1:A:210:VAL:HG22	1:B:627:GLN:HG2	1.88	0.56
1:B:201:ILE:HG22	1:B:212:LEU:CA	2.34	0.56
1:B:640:GLN:HA	1:B:643:TYR:HD1	1.70	0.56
1:B:147:LEU:HB3	1:B:155:ARG:HH22	1.69	0.56
2:D:626:THR:OG1	2:D:629:LEU:CG	2.53	0.56
1:A:600:LYS:O	1:A:608:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:THR:HG21	1:A:543:PRO:HG3	1.88	0.56
1:B:700:VAL:HB	1:B:709:LEU:HD13	1.87	0.56
2:C:340:LYS:CD	2:C:341:PRO:HD2	2.35	0.56
1:A:191:GLN:OE1	1:A:223:SER:N	2.39	0.56
1:B:210:VAL:HG13	1:B:211:TYR:CD2	2.40	0.56
2:D:626:THR:OG1	2:D:629:LEU:CD1	2.53	0.56
1:A:690:VAL:HG11	1:A:707:HIS:ND1	2.21	0.56
1:A:640:GLN:HA	1:A:643:TYR:CD1	2.37	0.55
2:C:158:CYS:HB2	2:C:173:LEU:HB2	1.88	0.55
2:C:188:TYR:CE1	2:C:206:LYS:HB2	2.41	0.55
2:C:347:LEU:HD23	2:C:377:CYS:SG	2.47	0.55
2:D:68:TYR:O	2:D:72:LEU:HG	2.05	0.55
2:C:371:ALA:HB3	2:C:377:CYS:SG	2.46	0.55
2:C:128:TRP:O	2:C:132:ILE:HB	2.06	0.55
1:B:210:VAL:CG1	1:B:211:TYR:CD2	2.89	0.55
2:C:121:GLY:HA2	2:C:160:PRO:HD2	1.89	0.55
1:B:305:THR:HG21	1:B:543:PRO:HG3	1.88	0.55
2:D:7:ARG:HA	2:D:38:ALA:HB3	1.89	0.55
2:C:626:THR:OG1	2:C:629:LEU:HD11	2.06	0.55
1:B:685:PHE:O	1:B:700:VAL:HG22	2.07	0.55
1:A:689:TYR:CG	1:A:737:LEU:HD22	2.41	0.55
1:A:635:MET:O	1:A:637:LEU:N	2.38	0.55
2:C:29:VAL:HG23	2:C:30:ILE:CD1	2.37	0.54
1:B:479:PHE:O	1:B:551:PRO:HD2	2.06	0.54
2:D:392:ASP:HB3	2:D:585:HIS:CE1	2.42	0.54
1:B:498:ALA:HB2	1:B:553:VAL:HA	1.90	0.54
2:D:321:THR:HG22	2:D:325:ASN:ND2	2.23	0.54
1:A:225:ALA:HA	1:A:377:VAL:HB	1.89	0.54
1:B:141:THR:HG22	1:B:584:ASN:HD22	1.71	0.54
2:D:626:THR:OG1	2:D:629:LEU:HD11	2.08	0.54
1:B:417:ALA:HA	1:B:421:VAL:HG23	1.88	0.54
2:D:596:CYS:O	2:D:600:ILE:HG12	2.08	0.54
2:C:124:ARG:HH12	2:C:187:GLY:HA2	1.72	0.53
1:A:210:VAL:HG12	1:A:211:TYR:CD2	2.43	0.53
1:A:223:SER:CB	1:A:379:ASN:ND2	2.68	0.53
1:B:130:LYS:HD2	1:B:440:ASP:OD2	2.09	0.53
1:B:489:LEU:HD12	1:B:556:CYS:SG	2.49	0.53
1:A:210:VAL:CG1	1:A:211:TYR:CD2	2.91	0.53
1:B:200:VAL:HG13	1:B:200:VAL:O	2.08	0.53
1:B:523:TYR:OH	1:B:526:SER:HA	2.08	0.53
2:D:217:LYS:HA	2:D:220:ARG:HE	1.71	0.53
1:A:408:GLN:O	1:A:419:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:PHE:CE2	1:B:299:GLY:HA3	2.44	0.53
1:B:307:ASP:N	1:B:461:VAL:HG13	2.24	0.53
1:B:232:LEU:HA	1:B:254:ILE:O	2.08	0.53
1:A:503:TYR:HD2	1:A:613:ARG:HD2	1.73	0.53
1:A:562:ASP:N	1:A:562:ASP:OD2	2.41	0.53
1:A:597:PHE:O	1:A:601:LEU:CG	2.56	0.53
2:C:671:LEU:HD13	2:C:671:LEU:O	2.08	0.53
2:D:627:LYS:HA	2:D:633:ASP:OD2	2.09	0.53
2:C:293:LEU:O	2:C:295:PHE:N	2.42	0.53
1:B:214:GLU:O	1:B:216:PRO:HD3	2.09	0.52
2:C:83:GLU:HG2	2:C:249:HIS:O	2.09	0.52
2:C:34:GLY:N	2:C:35:PRO:CD	2.67	0.52
1:A:512:ASN:O	1:A:512:ASN:ND2	2.28	0.52
1:B:515:HIS:ND1	1:B:516:PRO:HD2	2.25	0.52
1:A:476:LEU:O	1:A:679:MET:HE1	2.10	0.52
2:C:353:LEU:HD23	2:C:353:LEU:O	2.09	0.52
1:A:316:PHE:C	1:A:318:HIS:N	2.62	0.52
1:B:573:TYR:O	1:B:577:ILE:HG22	2.09	0.52
2:D:611:ASP:OD1	2:D:612:VAL:N	2.42	0.52
1:A:692:PRO:HG3	1:A:698:ARG:HD3	1.90	0.52
1:B:392:VAL:HG22	1:B:393:ILE:N	2.24	0.52
1:B:623:ARG:HD3	2:D:363:VAL:HG22	1.91	0.52
1:A:515:HIS:ND1	1:A:516:PRO:HD2	2.25	0.52
1:B:254:ILE:HD12	1:B:373:VAL:HG23	1.91	0.52
1:A:543:PRO:O	1:A:547:TYR:HB3	2.09	0.52
1:B:252:GLY:HA2	1:B:277:ILE:HD11	1.91	0.51
1:A:700:VAL:HG23	1:A:701:PHE:CD1	2.45	0.51
2:C:105:SER:H	2:C:232:ARG:HH12	1.57	0.51
1:A:516:PRO:HG3	1:A:586:VAL:HG22	1.93	0.51
1:A:232:LEU:HA	1:A:254:ILE:O	2.10	0.51
1:B:489:LEU:HB2	1:B:558:CYS:HA	1.91	0.51
2:C:173:LEU:HD23	2:C:194:CYS:SG	2.51	0.51
2:C:26:MET:SD	2:C:30:ILE:CD1	2.99	0.51
1:A:642:LEU:HD11	1:A:735:LEU:HD11	1.92	0.51
1:A:239:THR:HA	1:A:262:ILE:HD13	1.93	0.51
1:A:386:ILE:HG23	1:A:454:SER:HB3	1.93	0.51
2:C:128:TRP:CE2	2:C:132:ILE:HG13	2.46	0.51
1:A:143:THR:OG1	1:A:428:LYS:HE3	2.10	0.50
1:B:393:ILE:CD1	1:B:450:PHE:HE1	2.24	0.50
2:D:333:GLU:HG2	2:D:334:ALA:N	2.26	0.50
1:B:647:GLY:O	1:B:651:ARG:HG3	2.10	0.50
1:A:621:PHE:CG	1:A:709:LEU:HD23	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:402:TYR:HA	1:B:447:SER:O	2.11	0.50
2:C:210:ILE:HG12	2:C:235:VAL:HG11	1.94	0.50
1:A:219:TYR:HA	1:A:335:GLN:HE22	1.76	0.50
1:B:295:LEU:HD22	1:B:570:MET:CE	2.42	0.50
1:A:480:THR:HA	1:A:551:PRO:O	2.12	0.50
2:C:11:VAL:O	2:C:12:SER:CB	2.60	0.50
1:B:515:HIS:CG	1:B:516:PRO:HD2	2.47	0.50
2:C:80:VAL:HG23	2:C:81:VAL:N	2.26	0.50
1:A:258:ARG:HG2	1:A:282:TYR:CZ	2.47	0.50
1:A:597:PHE:O	1:A:601:LEU:HD12	2.12	0.49
1:A:512:ASN:C	1:A:512:ASN:ND2	2.65	0.49
1:A:214:GLU:HG2	1:A:215:ASN:N	2.27	0.49
2:C:96:TYR:HB2	2:C:207:HIS:CD2	2.46	0.49
2:C:131:PRO:HB3	2:C:204:PHE:CD1	2.47	0.49
2:D:361:ASN:HB3	2:D:608:PHE:CZ	2.47	0.49
1:A:222:TYR:CE2	1:A:302:HIS:HB2	2.47	0.49
1:B:202:ILE:O	1:B:209:LEU:O	2.30	0.49
2:D:321:THR:HG22	2:D:325:ASN:HD21	1.77	0.49
1:A:262:ILE:O	1:A:267:LYS:HE2	2.12	0.49
1:A:154:PRO:O	1:A:161:LYS:CB	2.60	0.48
1:A:272:GLU:HG3	1:A:332:ILE:HD11	1.94	0.48
1:A:298:PHE:CG	1:A:299:GLY:N	2.82	0.48
1:B:699:HIS:O	1:B:708:THR:HG22	2.14	0.48
1:B:446:ARG:HD2	1:B:479:PHE:CZ	2.49	0.48
1:A:366:VAL:CG1	1:A:367:THR:N	2.76	0.48
2:C:127:GLY:O	2:C:131:PRO:HG3	2.13	0.48
1:A:685:PHE:CD2	1:A:701:PHE:HE1	2.31	0.48
2:C:124:ARG:NH1	2:C:187:GLY:HA2	2.29	0.48
2:D:188:TYR:CZ	5:D:905:CO3:C	2.97	0.48
2:C:161:CYS:N	2:C:179:CYS:SG	2.78	0.48
1:B:579:ARG:HH11	1:B:579:ARG:HB3	1.78	0.48
1:B:470:TYR:HB3	1:B:473:SER:HB3	1.95	0.48
1:B:625:LEU:HD23	1:B:642:LEU:HD13	1.95	0.48
1:A:685:PHE:CE2	1:A:701:PHE:HE1	2.32	0.47
2:C:130:ILE:N	2:C:131:PRO:CD	2.77	0.47
1:A:510:MET:HE1	1:A:522:LEU:HB3	1.96	0.47
2:D:308:ARG:HB2	2:D:669:SER:HB2	1.96	0.47
1:B:236:ASN:O	1:B:257:VAL:HA	2.14	0.47
1:B:475:HIS:CE1	1:B:476:LEU:HG	2.49	0.47
1:B:256:ILE:CG1	1:B:282:TYR:HD2	2.28	0.47
2:C:126:ALA:O	2:C:131:PRO:HD3	2.13	0.47
1:A:259:ALA:HA	1:A:267:LYS:CE	2.33	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:390:PHE:HE2	1:B:453:TRP:CH2	2.32	0.47
1:B:753:VAL:HG12	1:B:754:TRP:CE3	2.48	0.47
1:A:259:ALA:HB2	1:A:281:ILE:CG2	2.44	0.47
1:B:388:ASN:HB3	1:B:390:PHE:CZ	2.49	0.47
1:B:444:PRO:HB3	1:B:602:THR:CG2	2.43	0.47
2:C:594:GLU:O	2:C:598:HIS:HB2	2.13	0.47
2:C:18:LYS:CG	2:C:294:LEU:HD13	2.45	0.47
1:A:731:PHE:HA	1:A:734:GLN:HE21	1.80	0.47
1:A:751:GLY:O	1:A:755:ASP:CA	2.63	0.47
1:B:446:ARG:H	1:B:602:THR:HG23	1.79	0.47
2:D:400:GLY:HA3	2:D:647:TYR:HB3	1.96	0.47
1:A:494:PHE:HE2	1:A:510:MET:SD	2.37	0.47
1:B:201:ILE:HG22	1:B:212:LEU:CB	2.44	0.47
1:A:272:GLU:HG3	1:A:332:ILE:HD12	1.97	0.47
2:D:69:ASP:HA	2:D:72:LEU:CD1	2.45	0.47
1:B:433:PHE:O	1:B:437:VAL:HG23	2.14	0.47
1:B:542:PHE:N	1:B:543:PRO:CD	2.78	0.46
1:B:582:GLU:CD	1:B:582:GLU:H	2.19	0.46
1:B:182:TRP:CZ3	1:B:392:VAL:HG12	2.39	0.46
1:B:703:GLY:O	1:B:708:THR:HG21	2.15	0.46
1:A:434:SER:O	1:A:438:LEU:HD23	2.15	0.46
1:B:619:LEU:HD12	1:B:646:ARG:HH21	1.81	0.46
1:B:513:VAL:HG22	1:B:592:GLU:HG2	1.96	0.46
1:B:234:HIS:CE1	1:B:236:ASN:HA	2.50	0.46
2:C:192:PHE:CZ	2:C:210:ILE:HD12	2.50	0.46
1:A:155:ARG:C	1:A:411:ALA:O	2.46	0.46
1:A:220:VAL:HG23	1:A:336:THR:HG23	1.96	0.46
1:A:652:ALA:HB1	1:A:749:LEU:HB3	1.97	0.46
2:D:341:PRO:HA	2:D:365:LYS:O	2.15	0.46
2:C:406:PRO:HA	2:C:588:VAL:HA	1.96	0.46
1:B:260:GLY:O	1:B:261:LYS:HB3	2.15	0.46
1:A:225:ALA:HB2	1:A:379:ASN:H	1.81	0.46
1:A:708:THR:HB	1:A:710:PRO:HD2	1.98	0.46
2:C:308:ARG:HB2	2:C:669:SER:HB2	1.97	0.46
2:C:5:THR:HA	2:C:36:SER:HB3	1.97	0.46
2:C:15:GLU:HG3	2:C:294:LEU:HD12	1.97	0.46
2:C:186:PHE:H	2:C:190:GLY:HA3	1.81	0.46
1:B:502:LEU:O	1:B:506:ILE:HG13	2.16	0.46
1:A:751:GLY:O	1:A:752:ASP:HB2	2.15	0.46
1:A:502:LEU:HD22	1:A:505:LEU:HD23	1.98	0.46
1:A:225:ALA:HA	1:A:377:VAL:CB	2.46	0.46
2:C:625:GLU:CG	2:C:629:LEU:HD21	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:VAL:CG2	1:A:336:THR:HG23	2.45	0.45
2:D:343:LYS:H	2:D:387:ASP:HB2	1.80	0.45
1:A:446:ARG:CZ	1:A:607:LEU:HD23	2.46	0.45
1:B:446:ARG:CD	1:B:479:PHE:CZ	2.99	0.45
1:B:678:VAL:O	1:B:681:VAL:HG23	2.17	0.45
1:A:190:ILE:HD13	1:A:384:ILE:HD13	1.98	0.45
1:B:501:LEU:HD12	1:B:551:PRO:HG3	1.98	0.45
1:A:448:ILE:HD13	1:A:598:VAL:HG11	1.98	0.45
2:D:655:TYR:O	2:D:659:VAL:HG22	2.15	0.45
1:A:510:MET:CE	1:A:522:LEU:HB3	2.46	0.45
1:A:394:LYS:HA	1:A:447:SER:OG	2.15	0.45
1:A:227:THR:HG23	1:A:376:THR:HB	1.98	0.45
2:D:363:VAL:O	2:D:363:VAL:HG12	2.16	0.45
2:D:176:GLY:O	2:D:177:CYS:HB2	2.15	0.45
1:A:496:VAL:HG13	1:A:496:VAL:O	2.15	0.45
2:C:227:CYS:SG	2:C:231:THR:HG23	2.57	0.45
1:B:391:GLY:O	1:B:450:PHE:N	2.32	0.45
1:A:392:VAL:HG23	1:A:448:ILE:O	2.16	0.45
2:C:612:VAL:HG12	2:C:613:THR:N	2.31	0.45
1:A:243:PHE:HB3	1:A:274:LEU:HD12	1.99	0.45
2:D:293:LEU:C	2:D:295:PHE:H	2.20	0.45
1:B:320:GLN:HA	1:B:320:GLN:HE21	1.82	0.45
2:C:68:TYR:HD2	2:C:327:ARG:NH1	2.14	0.45
2:D:350:HIS:HB2	2:D:629:LEU:HD21	1.97	0.44
2:D:130:ILE:N	2:D:131:PRO:CD	2.79	0.44
1:B:432:MET:O	1:B:436:MET:HG2	2.17	0.44
1:A:181:VAL:HG13	1:A:390:PHE:O	2.18	0.44
2:C:340:LYS:HB3	2:C:593:LYS:NZ	2.30	0.44
1:B:446:ARG:HD3	1:B:479:PHE:CE2	2.52	0.44
1:A:597:PHE:O	1:A:601:LEU:CD1	2.65	0.44
1:B:731:PHE:HA	1:B:734:GLN:HE21	1.81	0.44
1:B:392:VAL:CG2	1:B:393:ILE:N	2.79	0.44
1:A:599:ILE:O	1:A:603:HIS:HB3	2.14	0.44
2:D:331:CYS:HA	2:D:332:PRO:HD3	1.81	0.44
2:C:34:GLY:N	2:C:35:PRO:HD3	2.33	0.44
1:B:555:PHE:CZ	1:B:594:ALA:HB2	2.52	0.44
1:B:282:TYR:CD1	1:B:282:TYR:C	2.91	0.44
1:A:365:MET:C	1:A:366:VAL:HG23	2.38	0.44
2:D:344:TRP:CZ3	2:D:601:LEU:HD21	2.50	0.44
1:B:542:PHE:HB3	1:B:543:PRO:HD3	2.00	0.44
1:B:619:LEU:HD12	1:B:646:ARG:NH2	2.33	0.44
2:D:377:CYS:HB3	2:D:389:MET:SD	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:403:VAL:HG23	1:B:480:THR:O	2.17	0.44
1:A:706:SER:O	1:A:711:ALA:HB3	2.17	0.43
1:B:504:THR:OG1	1:B:613:ARG:NH2	2.49	0.43
2:D:128:TRP:C	2:D:131:PRO:HD2	2.38	0.43
1:B:232:LEU:HD22	1:B:373:VAL:HG11	1.99	0.43
1:A:573:TYR:O	1:A:577:ILE:HG22	2.19	0.43
1:A:493:ASN:HD21	1:A:495:LYS:HE3	1.83	0.43
2:D:186:PHE:H	2:D:190:GLY:HA3	1.83	0.43
1:A:278:GLY:HA2	1:A:332:ILE:HG23	1.99	0.43
1:A:551:PRO:HG3	1:A:682:GLU:HG2	2.00	0.43
1:B:708:THR:HB	1:B:710:PRO:HD2	2.01	0.43
1:A:154:PRO:O	1:A:161:LYS:HB2	2.18	0.43
1:A:238:GLY:C	1:A:262:ILE:HD11	2.39	0.43
1:A:384:ILE:HD12	1:A:386:ILE:HD11	2.00	0.43
1:B:515:HIS:ND1	1:B:516:PRO:CD	2.82	0.43
1:A:709:LEU:N	1:A:710:PRO:CD	2.82	0.43
2:C:96:TYR:H	2:C:207:HIS:CD2	2.36	0.43
1:A:223:SER:OG	1:A:377:VAL:HG11	2.18	0.43
1:B:256:ILE:CG1	1:B:282:TYR:CD2	3.02	0.43
2:C:411:ASN:HD21	2:C:422:PRO:HA	1.84	0.43
1:A:188:VAL:HG12	1:A:315:SER:OG	2.17	0.43
1:A:604:ASP:CG	1:A:605:VAL:H	2.21	0.43
1:A:222:TYR:CE2	1:A:302:HIS:CB	3.02	0.43
2:C:338:GLU:HA	2:C:338:GLU:OE1	2.17	0.43
1:A:250:VAL:HG12	1:A:250:VAL:O	2.19	0.43
1:B:537:LEU:H	1:B:537:LEU:HD12	1.83	0.43
2:C:80:VAL:O	2:C:305:VAL:HB	2.19	0.43
2:C:22:PHE:CE2	2:C:37:VAL:HG21	2.53	0.43
1:A:604:ASP:CG	1:A:605:VAL:N	2.72	0.43
2:D:63:ASP:O	2:D:67:VAL:HG23	2.19	0.43
2:D:12:SER:HB2	2:D:180:SER:HB2	2.00	0.43
1:B:298:PHE:CG	1:B:299:GLY:N	2.87	0.43
1:A:316:PHE:C	1:A:318:HIS:H	2.22	0.43
1:B:198:ASN:OD1	1:B:377:VAL:HA	2.19	0.43
2:D:343:LYS:HB2	2:D:387:ASP:OD2	2.19	0.43
2:C:612:VAL:HG12	2:C:613:THR:H	1.83	0.43
1:B:649:PHE:O	1:B:653:THR:HG23	2.19	0.43
2:D:262:LEU:HD23	2:D:262:LEU:O	2.19	0.43
2:C:94:PHE:CG	2:C:94:PHE:O	2.72	0.43
1:B:282:TYR:CD1	1:B:282:TYR:O	2.72	0.43
2:C:391:LEU:HD12	2:C:588:VAL:CG2	2.48	0.43
1:A:122:LEU:N	1:A:122:LEU:HD12	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:ILE:O	1:B:297:PHE:HZ	2.03	0.42
1:B:461:VAL:O	1:B:465:GLU:HG2	2.19	0.42
2:D:615:CYS:CA	2:D:618:ASN:O	2.65	0.42
2:C:676:PHE:HD1	2:C:677:ARG:HG3	1.85	0.42
1:A:595:GLY:O	1:A:599:ILE:HG12	2.19	0.42
1:A:603:HIS:CD2	1:A:603:HIS:C	2.93	0.42
1:A:551:PRO:CG	1:A:682:GLU:HG2	2.49	0.42
2:C:37:VAL:HG22	2:C:266:LEU:HD21	2.00	0.42
2:C:22:PHE:HD2	2:C:37:VAL:HG11	1.84	0.42
1:B:155:ARG:HD3	1:B:409:ARG:O	2.18	0.42
1:B:214:GLU:C	1:B:216:PRO:HD3	2.40	0.42
1:B:752:ASP:HB3	1:B:753:VAL:H	1.65	0.42
1:A:225:ALA:O	1:A:377:VAL:O	2.38	0.42
1:B:511:GLN:H	1:B:511:GLN:HG2	1.52	0.42
2:D:127:GLY:C	2:D:131:PRO:HG3	2.40	0.42
1:A:667:ASP:HB3	1:A:670:VAL:HG12	2.00	0.42
1:B:169:VAL:HG12	1:B:173:PHE:CE1	2.54	0.42
2:C:160:PRO:O	2:C:161:CYS:HB2	2.20	0.42
1:A:314:PRO:HB2	1:A:316:PHE:CD2	2.54	0.42
1:B:232:LEU:HB2	1:B:373:VAL:CG2	2.50	0.42
2:C:373:THR:OG1	2:C:376:ASP:OD2	2.26	0.42
2:C:306:PRO:HA	2:C:307:PRO:HD3	1.84	0.42
2:C:128:TRP:O	2:C:132:ILE:HG12	2.19	0.42
1:A:495:LYS:O	1:A:556:CYS:N	2.50	0.42
1:B:425:LEU:CD2	1:B:591:ALA:HB2	2.50	0.42
1:A:251:ASN:OD1	1:A:251:ASN:C	2.58	0.42
1:B:182:TRP:HZ3	1:B:392:VAL:CG1	2.25	0.42
2:C:49:ILE:HD13	2:C:70:ALA:HB2	2.01	0.42
2:D:128:TRP:CH2	2:D:150:VAL:HG21	2.55	0.42
2:D:333:GLU:HG2	2:D:334:ALA:H	1.85	0.42
1:A:715:ASN:HD22	1:A:734:GLN:HE22	1.68	0.42
2:C:4:LYS:HE2	2:C:4:LYS:HB2	1.81	0.42
1:A:700:VAL:CG1	1:A:741:THR:HG21	2.50	0.41
1:A:630:ALA:O	1:A:634:GLU:HG3	2.19	0.41
1:B:182:TRP:CE2	1:B:390:PHE:HB2	2.55	0.41
1:B:156:GLU:O	1:B:162:ASP:HB2	2.20	0.41
2:C:132:ILE:HG22	2:C:326:LEU:HD11	2.02	0.41
2:C:676:PHE:CD1	2:C:677:ARG:HG3	2.54	0.41
2:D:586:ALA:HB2	2:D:650:TYR:CZ	2.55	0.41
1:B:376:THR:HG23	1:B:376:THR:O	2.20	0.41
1:A:686:LEU:HA	1:A:699:HIS:HA	2.01	0.41
1:B:392:VAL:HA	1:B:448:ILE:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:52:ILE:HD11	2:C:60:VAL:HG12	2.02	0.41
1:A:706:SER:HA	1:A:711:ALA:HB1	2.03	0.41
1:A:596:GLN:HB3	1:A:596:GLN:HE21	1.63	0.41
1:B:229:THR:HB	1:B:374:LYS:HG3	2.01	0.41
2:C:316:GLY:O	2:C:320:VAL:HG23	2.20	0.41
1:A:262:ILE:HG13	1:A:267:LYS:HG3	2.03	0.41
2:C:340:LYS:CB	2:C:593:LYS:NZ	2.82	0.41
1:B:173:PHE:HA	1:B:176:PHE:CD2	2.55	0.41
2:D:125:SER:O	2:D:130:ILE:HG12	2.21	0.41
1:B:433:PHE:HA	1:B:436:MET:HB2	2.02	0.41
2:C:361:ASN:HB3	2:C:608:PHE:CZ	2.55	0.41
1:B:500:PRO:HD2	1:B:702:TRP:CH2	2.56	0.41
1:A:691:SER:HA	1:A:692:PRO:HD3	1.91	0.41
2:C:363:VAL:O	2:C:363:VAL:HG12	2.21	0.41
2:D:378:ILE:O	2:D:382:MET:HG3	2.19	0.41
1:A:325:ARG:CG	1:A:329:LEU:HD12	2.50	0.41
1:A:640:GLN:HB2	2:C:353:LEU:HD21	2.03	0.41
2:D:344:TRP:CH2	2:D:631:PHE:CZ	3.09	0.41
1:B:143:THR:O	1:B:147:LEU:HG	2.20	0.41
2:D:11:VAL:O	2:D:12:SER:HB3	2.21	0.41
2:C:655:TYR:O	2:C:659:VAL:HG22	2.21	0.41
1:B:727:ASN:HB3	1:B:730:LEU:HB3	2.02	0.41
1:B:500:PRO:O	1:B:613:ARG:HG2	2.20	0.41
1:A:128:LYS:HE2	1:A:512:ASN:OD1	2.21	0.41
1:A:731:PHE:HA	1:A:734:GLN:NE2	2.36	0.41
1:A:230:GLY:O	1:A:372:ASN:HB2	2.21	0.41
1:A:619:LEU:HD23	1:A:619:LEU:O	2.20	0.41
1:B:219:TYR:HA	1:B:335:GLN:HE22	1.86	0.41
2:D:5:THR:HG22	2:D:36:SER:OG	2.20	0.41
1:B:537:LEU:N	1:B:537:LEU:HD12	2.36	0.41
1:B:442:PHE:CD2	1:B:444:PRO:HG3	2.55	0.40
2:C:128:TRP:O	2:C:132:ILE:CB	2.68	0.40
2:C:63:ASP:HB2	2:C:249:HIS:CE1	2.56	0.40
1:B:262:ILE:CD1	1:B:267:LYS:HG2	2.51	0.40
1:A:221:ALA:O	1:A:222:TYR:CB	2.68	0.40
1:A:314:PRO:HA	1:A:465:GLU:OE2	2.21	0.40
1:B:218:GLY:O	1:B:335:GLN:NE2	2.53	0.40
2:C:6:VAL:HG13	2:C:259:LYS:HZ1	1.86	0.40
2:C:5:THR:HG22	2:C:36:SER:OG	2.20	0.40
1:B:236:ASN:CG	1:B:237:PHE:H	2.23	0.40
1:A:236:ASN:CG	1:A:237:PHE:H	2.24	0.40
1:A:349:MET:HA	1:A:367:THR:HA	2.01	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:ILE:O	1:A:551:PRO:C	2.59	0.40
1:B:579:ARG:NH1	1:B:579:ARG:HB3	2.36	0.40
1:B:622:VAL:HG11	2:D:360:VAL:HG21	2.03	0.40
2:D:394:GLY:O	2:D:398:ILE:HG12	2.22	0.40
1:A:124:TRP:CE2	1:A:600:LYS:NZ	2.90	0.40
2:C:344:TRP:NE1	2:C:630:LEU:HD22	2.37	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	636/654 (97%)	589 (93%)	42 (7%)	5 (1%)	27	78
1	B	637/654 (97%)	594 (93%)	37 (6%)	6 (1%)	25	76
2	C	513/693 (74%)	474 (92%)	33 (6%)	6 (1%)	19	71
2	D	468/693 (68%)	437 (93%)	27 (6%)	4 (1%)	25	76
All	All	2254/2694 (84%)	2094 (93%)	139 (6%)	21 (1%)	25	76

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	629	LEU
2	C	55	ASN
1	A	210	VAL
1	A	251	ASN
1	A	475	HIS
2	C	34	GLY
1	A	330	PRO
1	B	210	VAL
2	D	76	ASN
1	B	225	ALA
2	C	12	SER
2	D	339	CYS

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Mol	Chain	Res	Type
1	A	154	PRO
2	C	339	CYS
1	B	415	GLY
1	B	636	GLY
2	C	609	GLY
1	B	190	ILE
2	C	306	PRO
2	D	609	GLY
1	B	688	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/562 (91%)	511 (100%)	1 (0%)	96	99
1	B	473/562 (84%)	471 (100%)	2 (0%)	95	98
2	C	357/585 (61%)	355 (99%)	2 (1%)	92	98
2	D	277/585 (47%)	277 (100%)	0	100	100
All	All	1619/2294 (71%)	1614 (100%)	5 (0%)	96	99

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	B	511	GLN
1	B	603	HIS
2	C	71	TYR
2	C	241	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	186	HIS
1	A	285	GLN
1	A	318	HIS
1	A	335	GLN
1	A	348	ASN
1	A	475	HIS
1	A	483	ASN
1	A	511	GLN
1	A	596	GLN
1	A	603	HIS
1	A	626	ASN
1	A	684	HIS
1	A	734	GLN
1	A	747	ASN
1	B	320	GLN
1	B	483	ASN
1	B	511	GLN
1	B	512	ASN
1	B	584	ASN
1	B	596	GLN
1	B	626	ASN
1	B	727	ASN
1	B	734	GLN
2	C	207	HIS
2	C	584	ASN
2	C	585	HIS
2	C	604	GLN
2	D	325	ASN
2	D	584	ASN
2	D	585	HIS
2	D	604	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	NAG	A	903	1	12,14,15	0.47	0	15,19,21	1.21	1 (6%)
3	NAG	B	903	1	12,14,15	0.47	0	15,19,21	1.21	1 (6%)
5	CO3	C	905	6	0,3,3	0.00	-	0,3,3	0.00	-
5	CO3	D	905	6	0,3,3	0.00	-	0,3,3	0.00	-

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	NAG	A	903	1	-	0/6/23/26	0/1/1/1
3	NAG	B	903	1	-	0/6/23/26	0/1/1/1
5	CO3	C	905	6	-	0/0/0/0	0/0/0/0
5	CO3	D	905	6	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	NAG	O5-C5-C6	2.38	109.48	106.98
3	A	903	NAG	O5-C5-C6	2.37	109.47	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	638/654 (97%)	-0.30	2 (0%)	91 63	28, 75, 122, 200	0
1	B	639/654 (97%)	-0.12	5 (0%)	83 39	42, 99, 173, 200	0
2	C	517/693 (74%)	0.01	3 (0%)	86 46	61, 116, 172, 200	0
2	D	488/693 (70%)	0.06	3 (0%)	86 46	66, 136, 182, 200	0
All	All	2282/2694 (84%)	-0.10	13 (0%)	86 46	28, 103, 175, 200	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	GLY	5.3
1	B	206	ASN	2.8
2	D	278	LYS	2.7
2	D	175	PRO	2.6
1	A	724	GLY	2.5
2	C	665	CYS	2.3
1	B	154	PRO	2.3
1	B	210	VAL	2.1
2	C	642	HIS	2.1
1	B	207	GLY	2.0
2	D	12	SER	2.0
2	C	658	ALA	2.0
1	A	758	ASN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	903	14/15	0.33	3.58	140,140,140,140	0
3	NAG	A	903	14/15	0.27	0.84	116,116,116,116	0
5	CO3	D	905	4/4	0.17	-0.10	127,127,127,127	0
6	FE	D	901	1/1	0.12	-1.23	163,163,163,163	0
4	CA	B	900	1/1	0.14	-1.47	80,80,80,80	0
4	CA	A	900	1/1	0.14	-1.49	61,61,61,61	0
6	FE	C	901	1/1	0.12	-2.46	118,118,118,118	0
5	CO3	C	905	4/4	0.10	-2.95	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.