



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 10:27 AM GMT

PDB ID : 1F6A
Title : Structure of the human ige-fc bound to its high affinity receptor
fc(epsilon)ri(alpha)
Authors : Garman, S.C.; Wurzburg, B.A.; Tarchevskaya, S.S.; Kinet, J.P.; Jardetzky,
T.S.
Deposited on : 2000-06-20
Resolution : 3.50 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>

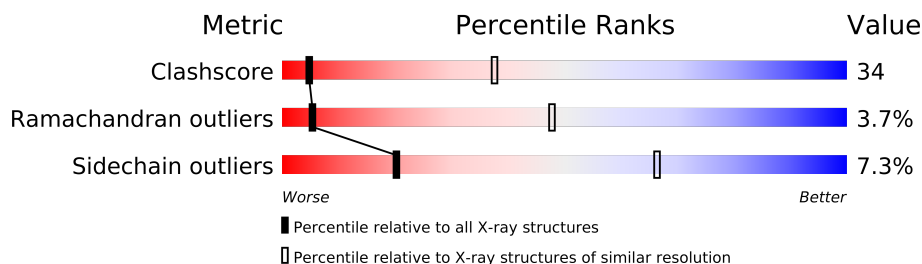
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 3.50 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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	176	
2	B	222	
2	D	222	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5251 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1406	902	229	270	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	ENGINEERED	UNP P12319
A	135	ALA	ASN	ENGINEERED	UNP P12319
A	142	ALA	THR	ENGINEERED	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319

- Molecule 2 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1711	1067	317	320	7			
2	D	216	Total	C	N	O	S	0	0	0
			1704	1062	316	319	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	326	ALA	-	CLONING ARTIFACT	UNP P01854
B	327	ASP	-	CLONING ARTIFACT	UNP P01854
B	328	PRO	-	CLONING ARTIFACT	UNP P01854
B	329	CYS	-	CLONING ARTIFACT	UNP P01854
D	326	ALA	-	CLONING ARTIFACT	UNP P01854
D	327	ASP	-	CLONING ARTIFACT	UNP P01854
D	328	PRO	-	CLONING ARTIFACT	UNP P01854
D	329	CYS	-	CLONING ARTIFACT	UNP P01854

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			49	28	2	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	ENGINEERED	UNP P12319
A	135	ALA	ASN	ENGINEERED	UNP P12319
A	142	ALA	THR	ENGINEERED	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	ENGINEERED	UNP P12319
A	135	ALA	ASN	ENGINEERED	UNP P12319
A	142	ALA	THR	ENGINEERED	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	ENGINEERED	UNP P12319
A	135	ALA	ASN	ENGINEERED	UNP P12319
A	142	ALA	THR	ENGINEERED	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	6	Total	C	N	O	0	0
			72	40	2	30		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	326	ALA	-	CLONING ARTIFACT	UNP P01854
B	327	ASP	-	CLONING ARTIFACT	UNP P01854
B	328	PRO	-	CLONING ARTIFACT	UNP P01854
B	329	CYS	-	CLONING ARTIFACT	UNP P01854

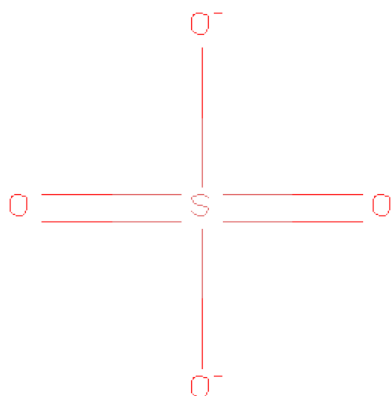
- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	3	Total	C	N	O	0	0
			39	22	2	15		

There are 4 discrepancies between the modelled and reference sequences:

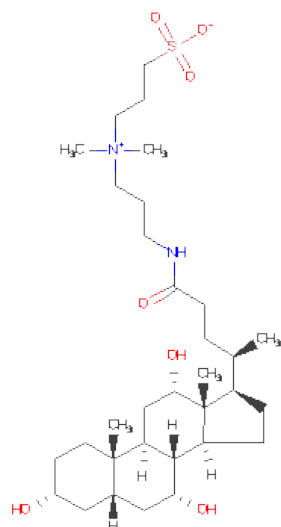
Chain	Residue	Modelled	Actual	Comment	Reference
D	326	ALA	-	CLONING ARTIFACT	UNP P01854
D	327	ASP	-	CLONING ARTIFACT	UNP P01854
D	328	PRO	-	CLONING ARTIFACT	UNP P01854
D	329	CYS	-	CLONING ARTIFACT	UNP P01854

- Molecule 8 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 9 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 26 23 3	0	0
9	A	1	Total C N O S 42 32 2 7 1	0	0
9	D	1	Total C O 26 23 3	0	0
9	D	1	Total C O 26 23 3	0	0
9	D	1	Total C O 26 23 3	0	0

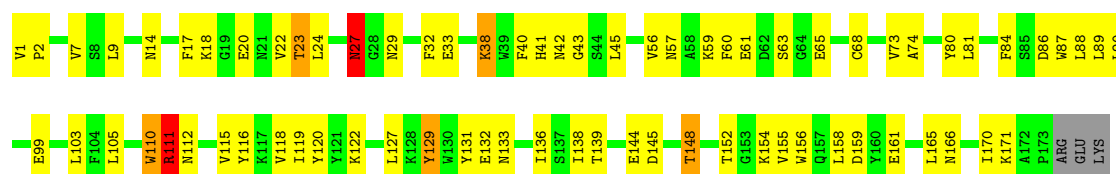
3 Residue-property plots

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.

Note EDS was not executed.

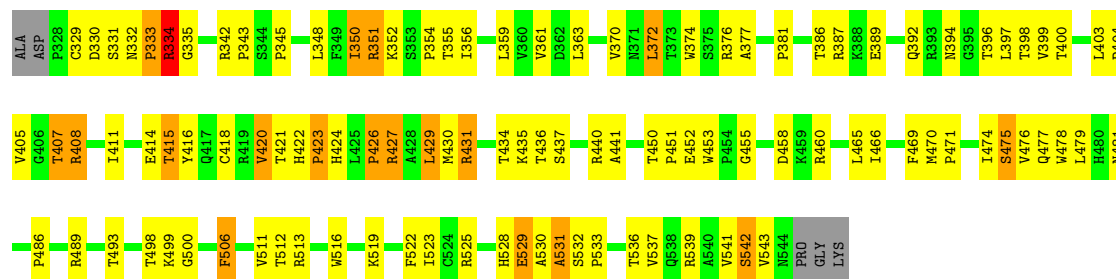
• Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT

Chain A: 



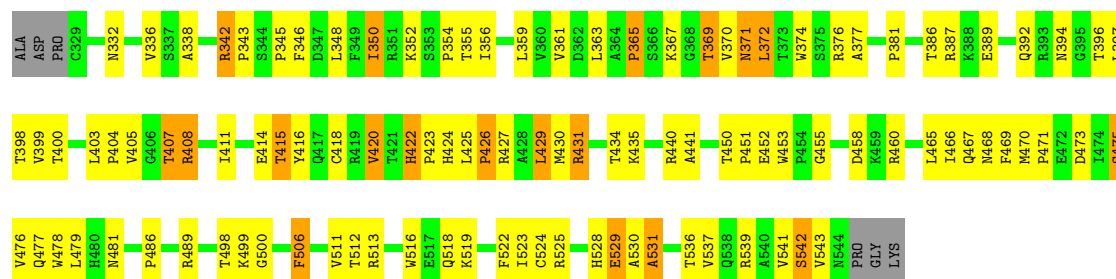
• Molecule 2: IG EPSILON CHAIN C REGION

Chain B: 



• Molecule 2: IG EPSILON CHAIN C REGION

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.80Å 192.80Å 302.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.87 – 3.50	Depositor
% Data completeness (in resolution range)	99.6 (36.87-3.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

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: FUC, CPS, NAG, SO4, MAN

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	0.50	0/1448	0.73	1/1974 (0.1%)
2	B	0.49	2/1755 (0.1%)	0.77	2/2389 (0.1%)
2	D	0.48	2/1747 (0.1%)	0.76	2/2378 (0.1%)
All	All	0.49	4/4950 (0.1%)	0.76	5/6741 (0.1%)

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
3	A	1	0
4	A	1	0
6	B	1	0
7	D	1	0
All	All	4	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	529	GLU	CD-OE1	-8.78	1.16	1.25
2	B	529	GLU	CD-OE1	-8.01	1.16	1.25
2	B	529	GLU	CD-OE2	-7.74	1.17	1.25
2	D	529	GLU	CD-OE2	-7.45	1.17	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	529	GLU	OE1-CD-OE2	-16.97	102.93	123.30
2	D	529	GLU	OE1-CD-OE2	-16.73	103.23	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	529	GLU	CG-CD-OE2	5.70	129.70	118.30
2	B	529	GLU	CG-CD-OE2	5.29	128.87	118.30
1	A	27	ASN	N-CA-C	5.24	125.15	111.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	223	MAN	C1
4	A	244	MAN	C1
6	B	696	MAN	C1
7	D	696	MAN	C1

There are no planarity outliers.

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	1406	0	1322	76	0
2	B	1711	0	1687	131	1
2	D	1704	0	1679	126	1
3	A	49	0	43	0	0
4	A	61	0	52	4	0
5	A	38	0	34	0	0
6	B	72	0	61	9	0
7	D	39	0	34	0	0
8	A	5	0	0	1	0
8	B	15	0	0	2	0
8	D	5	0	0	0	0
9	A	68	0	91	13	0
9	D	78	0	105	12	0
All	All	5251	0	5108	356	2

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 34.

All (356) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:371:CPS:C5	9:A:371:CPS:C10	1.75	1.65
9:D:105:CPS:C10	9:D:105:CPS:C5	1.75	1.58
9:A:371:CPS:N1	9:A:371:CPS:C25	1.67	1.50
6:B:696:MAN:H61	6:B:697:MAN:H3	1.41	1.00
1:A:115:VAL:HG22	1:A:155:VAL:HG22	1.49	0.92
2:B:333:PRO:HD2	2:B:429:LEU:HG	1.53	0.90
2:B:422:HIS:CD2	2:B:423:PRO:HD2	2.06	0.89
2:D:377:ALA:HB3	2:D:415:THR:HG23	1.54	0.88
2:B:415:THR:HB	2:B:434:THR:HG21	1.56	0.87
2:B:345:PRO:HB2	2:B:475:SER:HB2	1.55	0.87
2:B:377:ALA:HB3	2:B:415:THR:HG23	1.55	0.87
1:A:170:ILE:HG22	1:A:171:LYS:H	1.39	0.86
2:D:465:LEU:HB2	2:D:506:PHE:HE2	1.41	0.86
2:D:422:HIS:ND1	2:D:423:PRO:HD2	1.90	0.85
6:B:696:MAN:H61	6:B:697:MAN:C3	2.01	0.85
9:A:371:CPS:C10	9:A:371:CPS:C6	2.55	0.85
9:D:105:CPS:C10	9:D:105:CPS:C6	2.55	0.84
9:D:105:CPS:C10	9:D:105:CPS:C9	2.55	0.84
1:A:118:VAL:HG21	1:A:133:ASN:HA	1.60	0.84
1:A:105:LEU:HB2	1:A:136:ILE:HB	1.59	0.84
2:D:415:THR:HB	2:D:434:THR:HG21	1.59	0.84
2:B:389:GLU:HG2	2:B:399:VAL:HG22	1.61	0.83
9:A:371:CPS:C9	9:A:371:CPS:C10	2.56	0.82
2:B:465:LEU:HB2	2:B:506:PHE:HE2	1.42	0.82
1:A:110:TRP:NE1	1:A:111:ARG:HG3	1.93	0.82
2:B:331:SER:HB2	2:B:431:ARG:HH22	1.45	0.82
9:A:371:CPS:C4	9:A:371:CPS:C10	2.60	0.80
2:B:415:THR:HB	2:B:434:THR:CG2	2.12	0.80
2:D:389:GLU:HG2	2:D:399:VAL:HG22	1.64	0.79
9:D:105:CPS:C10	9:D:105:CPS:C4	2.60	0.79
2:D:541:VAL:HG22	2:D:542:SER:H	1.48	0.79
2:B:541:VAL:HG22	2:B:542:SER:H	1.46	0.79
2:B:426:PRO:HG2	2:B:427:ARG:H	1.47	0.78
1:A:40:PHE:CE2	1:A:45:LEU:HD12	2.18	0.78
1:A:99:GLU:HB2	1:A:170:ILE:O	1.84	0.77
2:D:415:THR:HB	2:D:434:THR:CG2	2.14	0.77
1:A:111:ARG:HB3	1:A:111:ARG:HH11	1.50	0.76
1:A:115:VAL:HG22	1:A:155:VAL:CG2	2.16	0.76
2:D:465:LEU:HB2	2:D:506:PHE:CE2	2.21	0.75
2:B:541:VAL:HG22	2:B:542:SER:N	2.03	0.74
1:A:116:TYR:CE2	9:A:371:CPS:H29	2.23	0.74
2:D:369:THR:HG22	2:D:370:VAL:H	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:452:GLU:HB3	2:D:460:ARG:HH21	1.53	0.73
1:A:115:VAL:HG12	1:A:118:VAL:HG22	1.71	0.73
2:B:435:LYS:HE2	2:B:529:GLU:OE1	1.89	0.72
2:D:541:VAL:HG22	2:D:542:SER:N	2.04	0.72
2:D:345:PRO:HB2	2:D:475:SER:HB2	1.71	0.72
2:B:465:LEU:HB2	2:B:506:PHE:CE2	2.23	0.71
2:B:452:GLU:HB3	2:B:460:ARG:HH21	1.54	0.71
1:A:170:ILE:HG22	1:A:171:LYS:N	2.05	0.71
2:D:408:ARG:N	2:D:408:ARG:HD3	2.05	0.71
2:B:415:THR:HA	2:B:434:THR:HG22	1.74	0.70
2:B:377:ALA:CB	2:B:415:THR:HG23	2.21	0.70
1:A:59:LYS:HZ3	1:A:60:PHE:HD1	1.40	0.70
2:D:377:ALA:CB	2:D:415:THR:HG23	2.20	0.69
2:B:430:MET:O	2:B:431:ARG:HG2	1.92	0.69
2:B:513:ARG:HA	2:B:516:TRP:CZ3	2.27	0.69
1:A:1:VAL:H2	1:A:2:PRO:HD2	1.57	0.69
2:B:408:ARG:HD3	2:B:408:ARG:N	2.06	0.69
6:B:696:MAN:C6	6:B:697:MAN:H5	2.23	0.68
2:B:465:LEU:HD12	2:B:466:ILE:N	2.07	0.68
2:D:430:MET:O	2:D:431:ARG:HG2	1.93	0.68
2:D:513:ARG:HA	2:D:516:TRP:CZ3	2.29	0.68
1:A:1:VAL:N	1:A:2:PRO:HD2	2.09	0.67
2:B:458:ASP:OD1	2:B:513:ARG:HD2	1.94	0.67
2:B:421:THR:O	2:B:421:THR:HG22	1.94	0.67
2:D:415:THR:HA	2:D:434:THR:HG22	1.73	0.67
2:D:458:ASP:OD1	2:D:513:ARG:HD2	1.94	0.67
9:A:371:CPS:C24	9:A:371:CPS:C25	2.67	0.67
1:A:1:VAL:N	1:A:2:PRO:CD	2.58	0.67
2:B:355:THR:HG22	2:B:404:PRO:HA	1.77	0.66
2:D:465:LEU:HD12	2:D:466:ILE:N	2.11	0.65
2:B:334:ARG:O	2:B:334:ARG:HG3	1.96	0.64
2:B:333:PRO:O	2:B:335:GLY:N	2.31	0.64
2:D:460:ARG:HH11	2:D:543:VAL:HG11	1.61	0.64
1:A:103:LEU:HD23	1:A:138:ILE:HD12	1.78	0.64
2:D:359:LEU:HD13	2:D:400:THR:HG22	1.79	0.64
2:B:486:PRO:HD2	2:B:489:ARG:HG3	1.80	0.63
2:B:359:LEU:HD13	2:B:400:THR:HG22	1.80	0.63
4:A:242:NAG:H61	4:A:243:NAG:N2	2.12	0.63
2:D:486:PRO:HD2	2:D:489:ARG:HG3	1.81	0.63
2:B:460:ARG:HH11	2:B:543:VAL:HG11	1.64	0.62
2:D:355:THR:HG22	2:D:404:PRO:HA	1.81	0.62
2:D:408:ARG:HD3	2:D:408:ARG:H	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:408:ARG:HD3	2:B:408:ARG:H	1.63	0.61
2:B:348:LEU:HD12	2:B:407:THR:HG23	1.82	0.61
2:B:513:ARG:HA	2:B:516:TRP:CE3	2.35	0.61
2:B:536:THR:HG22	2:B:537:VAL:N	2.16	0.60
2:D:528:HIS:HD2	2:D:530:ALA:H	1.49	0.60
6:B:694:NAG:H62	6:B:695:NAG:H83	1.84	0.60
2:D:338:ALA:O	2:D:431:ARG:HD2	2.02	0.60
2:B:506:PHE:CD1	2:D:506:PHE:HB3	2.37	0.59
2:B:470:MET:HA	2:B:471:PRO:O	2.01	0.59
2:D:348:LEU:HD12	2:D:407:THR:HG23	1.84	0.59
2:B:536:THR:O	2:B:537:VAL:HG23	2.03	0.59
1:A:41:HIS:C	1:A:43:GLY:H	2.05	0.59
2:D:470:MET:HA	2:D:471:PRO:O	2.02	0.59
2:D:422:HIS:ND1	2:D:423:PRO:CD	2.64	0.58
2:D:513:ARG:HA	2:D:516:TRP:CE3	2.37	0.58
2:B:370:VAL:HG22	2:B:387:ARG:NH2	2.18	0.58
2:D:528:HIS:CD2	2:D:529:GLU:N	2.71	0.58
2:B:343:PRO:HD3	2:B:356:ILE:HG22	1.86	0.58
2:D:536:THR:HG22	2:D:537:VAL:N	2.18	0.58
2:D:453:TRP:HD1	2:D:455:GLY:H	1.51	0.58
2:B:528:HIS:CD2	2:B:529:GLU:N	2.72	0.58
2:B:437:SER:HA	2:B:440:ARG:NH2	2.18	0.57
2:D:367:LYS:HE2	9:D:105:CPS:H21B	1.86	0.57
6:B:697:MAN:O3	6:B:699:MAN:H2	2.04	0.57
1:A:118:VAL:CG2	1:A:133:ASN:HA	2.33	0.57
2:B:453:TRP:HD1	2:B:455:GLY:H	1.51	0.57
1:A:27:ASN:ND2	1:A:29:ASN:HB2	2.20	0.57
2:D:424:HIS:CD2	2:D:424:HIS:N	2.70	0.57
2:B:403:LEU:HD12	2:B:404:PRO:HD2	1.85	0.57
2:D:528:HIS:CD2	2:D:530:ALA:H	2.23	0.57
2:D:403:LEU:HD12	2:D:404:PRO:HD2	1.86	0.57
2:D:424:HIS:NE2	9:D:105:CPS:H11B	2.19	0.56
2:D:398:THR:HG22	2:D:399:VAL:N	2.19	0.56
2:B:398:THR:HG22	2:B:399:VAL:N	2.20	0.56
2:D:336:VAL:HG21	2:D:363:LEU:HD23	1.86	0.56
1:A:40:PHE:CE2	1:A:45:LEU:CD1	2.89	0.56
2:B:528:HIS:HD2	2:B:530:ALA:H	1.53	0.56
2:B:506:PHE:HB3	2:D:506:PHE:CD1	2.40	0.56
2:B:516:TRP:HA	2:B:519:LYS:O	2.06	0.56
1:A:154:LYS:HA	1:A:158:LEU:O	2.05	0.56
1:A:119:ILE:HG12	1:A:129:TYR:HB2	1.88	0.56
1:A:110:TRP:CD1	1:A:111:ARG:HG3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:498:THR:C	2:D:500:GLY:H	2.09	0.55
2:B:331:SER:HB2	2:B:431:ARG:NH2	2.20	0.55
2:D:460:ARG:HH11	2:D:543:VAL:CG1	2.19	0.55
2:D:516:TRP:HA	2:D:519:LYS:O	2.06	0.55
2:D:435:LYS:HE2	2:D:529:GLU:OE2	2.05	0.55
1:A:154:LYS:HG2	1:A:159:ASP:OD1	2.06	0.55
2:B:522:PHE:O	2:B:541:VAL:HG12	2.07	0.55
2:B:477:GLN:HE22	2:B:525:ARG:HH21	1.55	0.55
1:A:22:VAL:HG22	1:A:23:THR:N	2.22	0.55
1:A:115:VAL:CG2	1:A:155:VAL:HG22	2.31	0.54
1:A:87:TRP:O	1:A:88:LEU:HD23	2.06	0.54
2:B:460:ARG:HH11	2:B:543:VAL:CG1	2.20	0.54
2:B:498:THR:C	2:B:500:GLY:H	2.10	0.54
4:A:242:NAG:H61	4:A:243:NAG:HN2	1.73	0.54
2:D:394:ASN:OD1	2:D:396:THR:HG22	2.08	0.54
2:B:333:PRO:HG3	2:B:427:ARG:CG	2.37	0.54
9:A:371:CPS:C7	9:A:371:CPS:C10	2.86	0.54
2:B:528:HIS:CD2	2:B:530:ALA:H	2.26	0.54
1:A:73:VAL:HG13	1:A:74:ALA:N	2.23	0.54
2:B:376:ARG:HD2	2:B:414:GLU:OE2	2.07	0.54
6:B:696:MAN:C6	6:B:697:MAN:C5	2.85	0.54
9:A:371:CPS:C8	9:A:371:CPS:C10	2.86	0.54
2:B:414:GLU:HG3	2:B:415:THR:N	2.23	0.53
1:A:116:TYR:CE2	9:A:371:CPS:C29	2.90	0.53
2:B:394:ASN:OD1	2:B:396:THR:HG22	2.08	0.53
2:B:348:LEU:HA	2:B:354:PRO:HG3	1.91	0.53
2:D:541:VAL:CG2	2:D:542:SER:H	2.20	0.53
6:B:696:MAN:H62	6:B:697:MAN:H5	1.89	0.53
2:D:525:ARG:HD2	2:D:536:THR:HG21	1.90	0.53
2:B:333:PRO:CD	2:B:429:LEU:HG	2.32	0.53
1:A:122:LYS:NZ	1:A:145:ASP:HA	2.22	0.53
1:A:156:TRP:CZ2	9:D:103:CPS:H11A	2.44	0.52
2:D:477:GLN:HE22	2:D:525:ARG:HH21	1.56	0.52
2:D:531:ALA:HB1	2:D:537:VAL:HG23	1.90	0.52
1:A:116:TYR:CD2	9:A:371:CPS:H29	2.43	0.52
2:B:531:ALA:HB1	2:B:537:VAL:HG23	1.91	0.52
1:A:120:TYR:CD1	1:A:136:ILE:HD11	2.43	0.52
2:D:450:THR:HG22	2:D:451:PRO:O	2.10	0.52
2:B:329:CYS:C	2:B:331:SER:H	2.12	0.52
2:D:536:THR:O	2:D:537:VAL:HG23	2.08	0.52
1:A:170:ILE:CG2	1:A:171:LYS:H	2.18	0.52
1:A:9:LEU:HD23	1:A:24:LEU:CD2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:THR:HG22	1:A:161:GLU:HG3	1.92	0.52
2:D:367:LYS:HG3	9:D:105:CPS:O4	2.09	0.52
2:D:398:THR:CG2	2:D:399:VAL:N	2.72	0.52
2:B:386:THR:CG2	2:B:387:ARG:N	2.73	0.52
2:B:450:THR:HG22	2:B:451:PRO:O	2.08	0.52
2:B:420:VAL:HG22	2:B:429:LEU:CB	2.40	0.52
2:B:415:THR:CB	2:B:434:THR:CG2	2.87	0.52
2:B:398:THR:CG2	2:B:399:VAL:N	2.73	0.52
2:B:372:LEU:HD11	2:B:418:CYS:SG	2.50	0.52
2:D:372:LEU:HD11	2:D:418:CYS:SG	2.50	0.51
2:D:376:ARG:HD3	2:D:416:TYR:CE2	2.46	0.51
2:D:376:ARG:HD2	2:D:414:GLU:OE2	2.11	0.51
2:B:541:VAL:CG2	2:B:542:SER:N	2.73	0.51
2:D:392:GLN:HB2	2:D:396:THR:HG22	1.92	0.51
1:A:155:VAL:O	1:A:156:TRP:HB2	2.11	0.51
2:B:541:VAL:CG2	2:B:542:SER:H	2.19	0.51
1:A:148:THR:HG22	1:A:166:ASN:OD1	2.09	0.51
1:A:86:ASP:OD1	1:A:87:TRP:N	2.38	0.51
1:A:132:GLU:OE1	2:B:334:ARG:NH1	2.42	0.51
2:D:522:PHE:O	2:D:541:VAL:HG12	2.10	0.51
2:B:477:GLN:NE2	2:B:525:ARG:HE	2.09	0.51
1:A:40:PHE:HE2	1:A:45:LEU:CD1	2.24	0.51
2:D:522:PHE:HB2	2:D:541:VAL:HG13	1.92	0.51
2:B:408:ARG:CD	2:B:408:ARG:H	2.24	0.51
2:D:476:VAL:HG12	2:D:477:GLN:N	2.26	0.50
2:D:408:ARG:CD	2:D:408:ARG:H	2.24	0.50
1:A:56:VAL:O	1:A:57:ASN:C	2.48	0.50
2:B:392:GLN:HB2	2:B:396:THR:HG22	1.92	0.50
2:B:528:HIS:CD2	2:B:529:GLU:H	2.29	0.50
2:D:525:ARG:HD2	2:D:536:THR:CG2	2.41	0.50
2:B:506:PHE:CE1	2:D:506:PHE:HB3	2.47	0.50
2:B:415:THR:CA	2:B:434:THR:HG22	2.40	0.50
2:B:350:ILE:O	2:B:352:LYS:HG3	2.11	0.50
2:B:530:ALA:O	2:B:531:ALA:O	2.30	0.50
2:D:530:ALA:O	2:D:531:ALA:O	2.30	0.50
1:A:41:HIS:C	1:A:43:GLY:N	2.65	0.50
2:B:525:ARG:HD2	2:B:536:THR:HG21	1.93	0.49
2:B:522:PHE:HB2	2:B:541:VAL:HG13	1.93	0.49
9:D:105:CPS:C10	9:D:105:CPS:C7	2.90	0.49
2:B:476:VAL:HG12	2:B:477:GLN:N	2.28	0.49
2:B:470:MET:HA	2:B:471:PRO:C	2.33	0.49
1:A:88:LEU:HD21	1:A:115:VAL:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:VAL:CG1	1:A:118:VAL:HG22	2.42	0.49
2:B:333:PRO:HG3	2:B:427:ARG:HG3	1.93	0.49
2:D:386:THR:CG2	2:D:387:ARG:N	2.75	0.49
1:A:1:VAL:HG12	1:A:1:VAL:O	2.13	0.49
2:B:407:THR:O	2:B:411:ILE:HG13	2.13	0.49
2:B:525:ARG:HD2	2:B:536:THR:CG2	2.43	0.49
2:D:414:GLU:HG3	2:D:415:THR:N	2.26	0.48
9:A:371:CPS:C8	9:A:371:CPS:H10	2.43	0.48
2:D:528:HIS:CD2	2:D:529:GLU:H	2.30	0.48
9:D:105:CPS:C10	9:D:105:CPS:C8	2.91	0.48
2:B:331:SER:O	2:B:429:LEU:HD21	2.13	0.48
2:B:420:VAL:HG22	2:B:429:LEU:HB3	1.94	0.48
2:B:415:THR:CB	2:B:434:THR:HG22	2.43	0.48
2:D:348:LEU:HA	2:D:354:PRO:HG3	1.96	0.48
2:D:407:THR:O	2:D:411:ILE:HG13	2.13	0.48
2:B:541:VAL:O	2:B:542:SER:HB3	2.14	0.48
2:D:408:ARG:N	2:D:408:ARG:CD	2.76	0.48
1:A:1:VAL:H3	1:A:2:PRO:CD	2.26	0.48
2:D:363:LEU:HB2	2:D:397:LEU:O	2.14	0.48
2:B:376:ARG:HD3	2:B:416:TYR:CE2	2.48	0.48
2:B:466:ILE:HD12	2:B:476:VAL:HG22	1.96	0.48
2:B:536:THR:CG2	2:B:537:VAL:N	2.76	0.48
1:A:73:VAL:CG1	1:A:74:ALA:N	2.77	0.48
2:D:350:ILE:O	2:D:352:LYS:HG3	2.12	0.48
2:D:477:GLN:NE2	2:D:525:ARG:HE	2.12	0.47
1:A:18:LYS:HD2	1:A:60:PHE:CE1	2.50	0.47
2:D:415:THR:CB	2:D:434:THR:HG22	2.44	0.47
2:D:343:PRO:HD3	2:D:356:ILE:HG22	1.96	0.47
2:B:511:VAL:HG12	2:B:512:THR:N	2.29	0.47
2:D:466:ILE:HD12	2:D:476:VAL:HG22	1.95	0.47
4:A:242:NAG:H62	4:A:243:NAG:H82	1.97	0.47
2:D:470:MET:HA	2:D:471:PRO:C	2.35	0.47
1:A:110:TRP:C	1:A:112:ASN:N	2.68	0.47
1:A:111:ARG:HB3	1:A:111:ARG:NH1	2.25	0.47
2:B:333:PRO:C	2:B:335:GLY:N	2.68	0.47
2:D:415:THR:CA	2:D:434:THR:HG22	2.40	0.47
2:B:465:LEU:HD12	2:B:465:LEU:C	2.35	0.47
2:D:541:VAL:O	2:D:542:SER:HB3	2.14	0.47
1:A:59:LYS:HG3	1:A:60:PHE:N	2.30	0.47
2:D:441:ALA:HB3	2:D:470:MET:HG2	1.97	0.47
2:B:479:LEU:HB2	2:B:523:ILE:HB	1.97	0.47
2:B:414:GLU:CG	2:B:415:THR:N	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:493:THR:HB	8:B:204:SO4:O3	2.14	0.47
2:D:411:ILE:O	2:D:435:LYS:HE3	2.15	0.47
2:D:336:VAL:CG2	2:D:363:LEU:HD23	2.44	0.47
1:A:17:PHE:CE2	1:A:89:LEU:HB2	2.51	0.46
1:A:110:TRP:CD1	2:D:426:PRO:HG3	2.50	0.46
2:B:426:PRO:HG2	2:B:427:ARG:N	2.23	0.46
2:B:477:GLN:HE21	2:B:525:ARG:HE	1.63	0.46
2:D:415:THR:CB	2:D:434:THR:CG2	2.89	0.46
1:A:40:PHE:HE2	1:A:45:LEU:HD12	1.74	0.46
2:B:511:VAL:CG1	2:B:512:THR:N	2.79	0.46
1:A:17:PHE:CE1	1:A:110:TRP:HA	2.50	0.46
2:D:536:THR:CG2	2:D:537:VAL:N	2.79	0.46
2:B:426:PRO:CG	2:B:427:ARG:H	2.23	0.46
2:D:405:VAL:HG22	2:D:416:TYR:CZ	2.51	0.45
2:D:541:VAL:CG2	2:D:542:SER:N	2.74	0.45
1:A:32:PHE:O	1:A:33:GLU:HB2	2.16	0.45
2:D:511:VAL:HG12	2:D:512:THR:N	2.31	0.45
6:B:696:MAN:H61	6:B:697:MAN:C5	2.46	0.45
2:D:345:PRO:HD2	2:D:475:SER:OG	2.17	0.45
9:A:370:CPS:H11A	9:A:371:CPS:H11A	1.98	0.45
2:D:528:HIS:HD2	2:D:529:GLU:N	2.14	0.45
2:B:333:PRO:C	2:B:335:GLY:H	2.19	0.45
2:D:423:PRO:HB2	2:D:424:HIS:CD2	2.52	0.45
2:B:441:ALA:HB3	2:B:470:MET:HG2	1.99	0.45
2:D:522:PHE:HB2	2:D:541:VAL:CG1	2.47	0.45
1:A:41:HIS:O	1:A:43:GLY:N	2.50	0.45
2:D:479:LEU:HB2	2:D:523:ILE:HB	1.99	0.45
2:D:478:TRP:CZ3	2:D:524:CYS:HB2	2.52	0.45
2:D:420:VAL:HG22	2:D:429:LEU:CB	2.47	0.45
2:B:345:PRO:HG2	2:B:474:ILE:C	2.37	0.44
1:A:103:LEU:HB3	1:A:138:ILE:HB	1.98	0.44
2:D:414:GLU:CG	2:D:415:THR:N	2.80	0.44
2:B:528:HIS:HD2	2:B:529:GLU:N	2.13	0.44
2:B:424:HIS:NE2	8:B:202:SO4:O1	2.36	0.44
2:D:369:THR:HG22	2:D:370:VAL:N	2.27	0.44
2:B:332:ASN:N	2:B:333:PRO:HD3	2.32	0.44
2:B:411:ILE:O	2:B:435:LYS:HE3	2.16	0.44
2:B:374:TRP:CD2	2:B:403:LEU:HD22	2.52	0.44
2:B:403:LEU:HD12	2:B:404:PRO:CD	2.48	0.44
2:D:486:PRO:O	2:D:489:ARG:HB2	2.18	0.44
2:B:396:THR:HG23	2:B:397:LEU:N	2.32	0.44
2:B:405:VAL:HG22	2:B:416:TYR:CZ	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:D:105:CPS:C8	9:D:105:CPS:H10	2.48	0.44
6:B:696:MAN:H61	6:B:697:MAN:H5	1.98	0.44
1:A:63:SER:HA	1:A:81:LEU:O	2.18	0.44
2:B:450:THR:HA	2:B:451:PRO:HD3	1.75	0.43
2:D:396:THR:HG23	2:D:397:LEU:N	2.33	0.43
2:D:332:ASN:O	2:D:332:ASN:OD1	2.35	0.43
2:D:465:LEU:HD12	2:D:465:LEU:C	2.39	0.43
1:A:99:GLU:OE2	1:A:171:LYS:HG2	2.18	0.43
2:D:511:VAL:CG1	2:D:512:THR:N	2.81	0.43
2:B:469:PHE:HD1	2:B:528:HIS:CE1	2.37	0.43
2:D:460:ARG:NH1	2:D:543:VAL:HG11	2.32	0.43
4:A:244:MAN:O2	4:A:245:MAN:H5	2.18	0.43
1:A:110:TRP:CG	2:D:426:PRO:HG3	2.54	0.43
2:B:522:PHE:HB2	2:B:541:VAL:CG1	2.48	0.43
2:B:437:SER:HA	2:B:440:ARG:HH22	1.83	0.43
2:D:476:VAL:CG1	2:D:477:GLN:N	2.82	0.43
2:D:450:THR:HA	2:D:451:PRO:HD3	1.78	0.42
2:D:478:TRP:O	2:D:479:LEU:HD23	2.19	0.42
1:A:65:GLU:HB2	1:A:80:TYR:CE2	2.54	0.42
2:D:374:TRP:CD2	2:D:403:LEU:HD22	2.53	0.42
2:B:440:ARG:HD3	2:B:471:PRO:HD3	2.02	0.42
1:A:65:GLU:HB2	1:A:80:TYR:HE2	1.83	0.42
2:B:486:PRO:O	2:B:489:ARG:HB2	2.19	0.42
1:A:144:GLU:HG3	1:A:145:ASP:N	2.34	0.42
2:D:422:HIS:HB3	2:D:425:LEU:HD12	2.02	0.42
2:D:477:GLN:HE21	2:D:525:ARG:HE	1.67	0.42
2:D:403:LEU:HD12	2:D:404:PRO:CD	2.50	0.42
2:B:332:ASN:O	2:B:333:PRO:C	2.56	0.42
2:D:469:PHE:HD1	2:D:528:HIS:CE1	2.38	0.42
2:D:450:THR:HG22	2:D:451:PRO:N	2.35	0.42
2:B:450:THR:HG22	2:B:451:PRO:N	2.35	0.42
1:A:90:LEU:HD23	1:A:165:LEU:HB3	2.01	0.42
2:D:338:ALA:C	2:D:431:ARG:HD2	2.40	0.41
2:D:440:ARG:HD3	2:D:471:PRO:HD3	2.02	0.41
2:B:532:SER:HB3	2:B:533:PRO:HA	2.02	0.41
9:D:105:CPS:H19	9:D:105:CPS:H14	2.00	0.41
2:D:467:GLN:NE2	2:D:468:ASN:HD21	2.18	0.41
1:A:131:TYR:CG	2:B:334:ARG:HG2	2.55	0.41
1:A:41:HIS:HE1	1:A:63:SER:O	2.03	0.41
1:A:17:PHE:O	1:A:20:GLU:HG3	2.21	0.41
2:B:478:TRP:O	2:B:479:LEU:HD23	2.20	0.41
1:A:139:THR:OG1	8:A:203:SO4:O4	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:348:LEU:HD13	2:B:354:PRO:CG	2.50	0.41
2:B:330:ASP:O	2:B:330:ASP:OD1	2.39	0.41
2:D:420:VAL:HG22	2:D:429:LEU:HB3	2.02	0.41
1:A:84:PHE:N	1:A:84:PHE:CD1	2.88	0.41
1:A:59:LYS:HG2	1:A:61:GLU:OE1	2.21	0.41
2:D:348:LEU:HD13	2:D:354:PRO:CG	2.51	0.41
2:B:460:ARG:NH1	2:B:543:VAL:HG11	2.34	0.41
1:A:129:TYR:CD2	1:A:129:TYR:C	2.94	0.41
2:B:506:PHE:HB3	2:D:506:PHE:CE1	2.55	0.41
2:D:342:ARG:HD2	2:D:473:ASP:OD1	2.20	0.41
2:D:342:ARG:CD	2:D:473:ASP:OD1	2.68	0.40
2:D:370:VAL:O	2:D:371:ASN:C	2.60	0.40
2:B:498:THR:C	2:B:500:GLY:N	2.75	0.40
2:D:346:PHE:C	2:D:348:LEU:H	2.25	0.40
1:A:14:ASN:O	1:A:81:LEU:HA	2.21	0.40
2:D:425:LEU:HA	2:D:426:PRO:HD3	1.87	0.40
2:B:363:LEU:HB2	2:B:397:LEU:O	2.22	0.40
1:A:38:LYS:O	1:A:68:CYS:HA	2.22	0.40
2:B:420:VAL:HG22	2:B:429:LEU:HB2	2.03	0.40
2:B:436:THR:O	2:B:440:ARG:NH1	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:518:GLN:OE1	2:D:518:GLN:OE1[11_566]	1.79	0.41
2:B:351:ARG:NH2	2:B:351:ARG:NH2[4_556]	2.12	0.08

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	171/176 (97%)	147 (86%)	20 (12%)	4 (2%)	10	60
2	B	215/222 (97%)	177 (82%)	29 (14%)	9 (4%)	4	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	214/222 (96%)	175 (82%)	30 (14%)	9 (4%)	4	43
All	All	600/620 (97%)	499 (83%)	79 (13%)	22 (4%)	5	48

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
2	B	334	ARG
2	B	531	ALA
2	D	426	PRO
2	D	531	ALA
2	B	426	PRO
2	D	371	ASN
2	B	350	ILE
2	D	350	ILE
2	D	369	THR
1	A	111	ARG
2	B	499	LYS
2	B	542	SER
2	D	365	PRO
2	D	499	LYS
2	D	542	SER
1	A	42	ASN
1	A	110	TRP
2	B	351	ARG
2	B	381	PRO
2	D	381	PRO
2	B	333	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	154/157 (98%)	147 (96%)	7 (4%)	38	83
2	B	192/195 (98%)	176 (92%)	16 (8%)	16	59
2	D	191/195 (98%)	175 (92%)	16 (8%)	16	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	537/547 (98%)	498 (93%)	39 (7%)	20	66

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	23	THR
1	A	38	LYS
1	A	111	ARG
1	A	127	LEU
1	A	129	TYR
1	A	148	THR
2	B	334	ARG
2	B	342	ARG
2	B	361	VAL
2	B	372	LEU
2	B	407	THR
2	B	408	ARG
2	B	415	THR
2	B	420	VAL
2	B	423	PRO
2	B	427	ARG
2	B	429	LEU
2	B	431	ARG
2	B	475	SER
2	B	481	ASN
2	B	506	PHE
2	B	539	ARG
2	D	342	ARG
2	D	361	VAL
2	D	365	PRO
2	D	372	LEU
2	D	407	THR
2	D	408	ARG
2	D	415	THR
2	D	420	VAL
2	D	422	HIS
2	D	427	ARG
2	D	429	LEU
2	D	431	ARG
2	D	475	SER
2	D	481	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	506	PHE
2	D	539	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	54	ASN
1	A	157	GLN
2	B	383	ASN
2	B	468	ASN
2	B	477	GLN
2	B	481	ASN
2	B	518	GLN
2	B	528	HIS
2	B	538	GLN
2	D	332	ASN
2	D	383	ASN
2	D	468	ASN
2	D	477	GLN
2	D	481	ASN
2	D	518	GLN
2	D	528	HIS
2	D	538	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 ⓘ

21 carbohydrates 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	NAG	A	221	1,3	12,14,15	0.49	0	15,19,21	0.82	1 (6%)
3	NAG	A	222	3	12,14,15	0.45	0	15,19,21	0.78	0
3	MAN	A	223	3	10,11,12	0.45	0	11,15,17	0.31	0
3	FUC	A	224	3	9,10,11	0.45	0	10,14,16	0.29	0
4	NAG	A	242	1,4	12,14,15	0.58	0	15,19,21	0.80	1 (6%)
4	NAG	A	243	4	12,14,15	0.59	0	15,19,21	0.89	1 (6%)
4	MAN	A	244	4	10,11,12	0.62	0	11,15,17	0.52	0
4	MAN	A	245	4	10,11,12	0.50	0	11,15,17	0.58	0
4	MAN	A	246	4	10,11,12	0.43	0	11,15,17	0.31	0
5	NAG	A	366	1,5	12,14,15	0.62	0	15,19,21	0.71	1 (6%)
5	NAG	A	367	5	12,14,15	0.47	0	15,19,21	0.65	0
5	FUC	A	369	5	9,10,11	0.41	0	10,14,16	0.39	0
6	NAG	B	694	2,6	12,14,15	0.42	0	15,19,21	0.77	0
6	NAG	B	695	6	12,14,15	0.68	0	15,19,21	0.77	0
6	MAN	B	696	6	10,11,12	0.64	0	11,15,17	1.20	1 (9%)
6	MAN	B	697	6	10,11,12	0.71	0	11,15,17	1.18	0
6	MAN	B	698	6	10,11,12	0.44	0	11,15,17	0.34	0
6	MAN	B	699	6	10,11,12	0.78	0	11,15,17	0.55	0
7	NAG	D	694	2,7	12,14,15	0.55	0	15,19,21	0.68	0
7	NAG	D	695	7	12,14,15	0.52	0	15,19,21	0.77	0
7	MAN	D	696	7	10,11,12	0.43	0	11,15,17	0.28	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	NAG	A	221	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	222	3	-	0/6/23/26	0/1/1/1
3	MAN	A	223	3	1/1/4/5	0/2/19/22	0/1/1/1
3	FUC	A	224	3	-	0/0/17/20	0/1/1/1
4	NAG	A	242	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	243	4	-	0/6/23/26	0/1/1/1
4	MAN	A	244	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	245	4	-	0/2/19/22	0/1/1/1
4	MAN	A	246	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	366	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	367	5	-	0/6/23/26	0/1/1/1
5	FUC	A	369	5	-	0/0/17/20	0/1/1/1
6	NAG	B	694	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	695	6	-	1/6/23/26	0/1/1/1
6	MAN	B	696	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	697	6	-	0/2/19/22	0/1/1/1
6	MAN	B	698	6	-	0/2/19/22	0/1/1/1
6	MAN	B	699	6	-	0/2/19/22	0/1/1/1
7	NAG	D	694	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	695	7	-	0/6/23/26	0/1/1/1
7	MAN	D	696	7	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	696	MAN	O5-C5-C6	3.08	110.21	106.98
3	A	221	NAG	C2-N2-C7	-2.38	119.10	123.09
4	A	242	NAG	C2-N2-C7	-2.28	119.27	123.09
5	A	366	NAG	C2-N2-C7	-2.13	119.51	123.09
4	A	243	NAG	C2-N2-C7	-2.12	119.53	123.09

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	696	MAN	C1
6	B	696	MAN	C1
3	A	223	MAN	C1
4	A	244	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	695	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry

10 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	$\# Z > 2$
8	SO4	A	203	-	4,4,4	0.71	0	6,6,6	0.24	0
9	CPS	A	370	-	29,29,45	6.20	18 (62%)	46,47,70	4.21	27 (58%)
9	CPS	A	371	-	45,45,45	4.68	23 (51%)	70,70,70	3.32	30 (42%)
8	SO4	B	201	-	4,4,4	0.57	0	6,6,6	0.12	0
8	SO4	B	202	-	4,4,4	0.32	0	6,6,6	0.19	0
8	SO4	B	204	-	4,4,4	0.78	0	6,6,6	0.42	0
9	CPS	D	103	-	29,29,45	6.80	20 (68%)	46,47,70	4.04	28 (60%)
9	CPS	D	104	-	29,29,45	6.64	18 (62%)	46,47,70	4.05	28 (60%)
9	CPS	D	105	-	29,29,45	6.91	17 (58%)	46,47,70	3.99	27 (58%)
8	SO4	D	205	-	4,4,4	0.80	0	6,6,6	0.25	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
8	SO4	A	203	-	-	0/0/0/0	0/0/0/0
9	CPS	A	370	-	-	0/6/71/90	0/0/4/4
9	CPS	A	371	-	-	1/25/90/90	0/0/4/4
8	SO4	B	201	-	-	0/0/0/0	0/0/0/0
8	SO4	B	202	-	-	0/0/0/0	0/0/0/0
8	SO4	B	204	-	-	0/0/0/0	0/0/0/0
9	CPS	D	103	-	-	0/6/71/90	0/0/4/4
9	CPS	D	104	-	-	0/6/71/90	0/0/4/4
9	CPS	D	105	-	-	0/6/71/90	0/0/4/4
8	SO4	D	205	-	-	0/0/0/0	0/0/0/0

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	103	CPS	C23-C22	-26.65	1.44	1.55
9	D	105	CPS	C23-C22	-26.30	1.44	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	104	CPS	C23-C22	-25.28	1.45	1.55
9	A	370	CPS	C23-C22	-22.87	1.46	1.55
9	A	371	CPS	C32-S	-13.37	1.54	1.78
9	D	103	CPS	O4-C4	-12.89	1.21	1.43
9	A	370	CPS	O4-C4	-12.70	1.21	1.43
9	A	371	CPS	C10-C5	12.68	1.75	1.54
9	D	105	CPS	C10-C5	12.63	1.75	1.54
9	D	104	CPS	O4-C4	-12.57	1.21	1.43
9	D	105	CPS	O4-C4	-12.47	1.21	1.43
9	A	371	CPS	O4-C4	-12.12	1.22	1.43
9	D	104	CPS	C10-C5	11.90	1.74	1.54
9	D	103	CPS	C10-C5	11.83	1.74	1.54
9	A	370	CPS	C10-C5	10.53	1.71	1.54
9	A	371	CPS	C25-N1	9.00	1.67	1.46
9	D	105	CPS	C18-C19	8.86	1.71	1.53
9	A	371	CPS	C5-C9	-8.45	1.41	1.55
9	D	105	CPS	C5-C9	-8.14	1.41	1.55
9	A	371	CPS	C18-C19	8.02	1.69	1.53
9	D	103	CPS	C5-C9	-7.77	1.42	1.55
9	D	104	CPS	C18-C19	7.60	1.69	1.53
9	D	105	CPS	C18-C17	7.28	1.65	1.53
9	D	103	CPS	C18-C19	7.27	1.68	1.53
9	D	104	CPS	C5-C9	-7.21	1.43	1.55
9	D	104	CPS	C18-C17	7.09	1.65	1.53
9	A	370	CPS	C5-C9	-6.77	1.43	1.55
9	A	370	CPS	C18-C19	6.72	1.67	1.53
9	A	370	CPS	C18-C17	6.70	1.64	1.53
9	A	371	CPS	C18-C17	6.61	1.64	1.53
9	A	370	CPS	C3-C4	6.42	1.65	1.53
9	A	371	CPS	C3-C4	6.08	1.64	1.53
9	D	103	CPS	C18-C17	6.07	1.63	1.53
9	D	103	CPS	O3-C17	-5.93	1.29	1.43
9	D	104	CPS	C3-C4	5.80	1.63	1.53
9	A	371	CPS	O2S-S	-5.27	1.33	1.45
9	A	371	CPS	C23-C24	-5.24	1.40	1.51
9	D	105	CPS	C3-C4	5.23	1.62	1.53
9	D	104	CPS	O3-C17	-5.20	1.31	1.43
9	A	370	CPS	O3-C17	-5.12	1.31	1.43
9	D	105	CPS	O3-C17	-5.10	1.31	1.43
9	D	103	CPS	C3-C4	5.08	1.62	1.53
9	A	371	CPS	O3-C17	-4.46	1.33	1.43
9	D	104	CPS	C8-C9	4.42	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	103	CPS	C16-C15	-4.31	1.46	1.53
9	D	105	CPS	C8-C9	4.28	1.64	1.54
9	A	371	CPS	C8-C7	4.23	1.66	1.54
9	D	103	CPS	C8-C9	4.12	1.64	1.54
9	D	105	CPS	C14-C15	4.10	1.60	1.53
9	A	370	CPS	C5-C4	-3.98	1.48	1.54
9	D	104	CPS	C16-C15	-3.94	1.47	1.53
9	A	370	CPS	C16-C15	-3.93	1.47	1.53
9	D	105	CPS	C8-C7	3.75	1.64	1.54
9	A	371	CPS	C16-C15	-3.72	1.47	1.53
9	D	104	CPS	O2-C13	3.67	1.55	1.43
9	D	105	CPS	O2-C13	3.61	1.54	1.43
9	A	370	CPS	O2-C13	3.58	1.54	1.43
9	A	370	CPS	C8-C9	3.56	1.62	1.54
9	D	105	CPS	C5-C4	-3.53	1.48	1.54
9	A	371	CPS	O2-C13	3.53	1.54	1.43
9	A	371	CPS	C14-C15	3.47	1.59	1.53
9	D	104	CPS	C14-C15	3.43	1.59	1.53
9	A	371	CPS	C8-C9	3.42	1.62	1.54
9	D	105	CPS	C14-C13	3.41	1.58	1.51
9	D	104	CPS	C8-C7	3.40	1.63	1.54
9	D	103	CPS	C8-C7	3.37	1.63	1.54
9	D	105	CPS	C20-C9	3.29	1.61	1.54
9	D	104	CPS	C5-C4	-3.22	1.49	1.54
9	A	370	CPS	C8-C7	3.15	1.63	1.54
9	D	103	CPS	O2-C13	3.09	1.53	1.43
9	D	103	CPS	C14-C15	3.08	1.59	1.53
9	A	371	CPS	C5-C6	-3.08	1.50	1.55
9	A	370	CPS	C14-C15	3.04	1.59	1.53
9	D	104	CPS	C14-C13	2.93	1.57	1.51
9	D	104	CPS	C20-C9	2.88	1.60	1.54
9	A	370	CPS	C14-C13	2.88	1.57	1.51
9	D	103	CPS	C20-C9	2.74	1.59	1.54
9	D	103	CPS	C5-C4	-2.72	1.50	1.54
9	A	370	CPS	C22-C20	2.67	1.60	1.52
9	D	105	CPS	C16-C15	-2.67	1.49	1.53
9	A	370	CPS	C7-C6	-2.64	1.48	1.54
9	A	371	CPS	C14-C13	2.53	1.56	1.51
9	A	370	CPS	C11-C2	2.51	1.59	1.54
9	D	103	CPS	C14-C13	2.45	1.56	1.51
9	D	103	CPS	C11-C2	2.40	1.59	1.54
9	A	371	CPS	C5-C4	-2.38	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	371	CPS	C20-C9	2.38	1.59	1.54
9	D	105	CPS	C11-C2	2.31	1.58	1.54
9	D	104	CPS	C22-C20	2.25	1.58	1.52
9	D	103	CPS	C7-C6	-2.22	1.49	1.54
9	A	371	CPS	C3-C19	-2.19	1.50	1.53
9	D	103	CPS	C5-C6	-2.19	1.51	1.55
9	A	371	CPS	C11-C2	2.07	1.58	1.54
9	D	103	CPS	C22-C20	2.07	1.58	1.52
9	A	371	CPS	C22-C23	-2.06	1.45	1.52
9	D	104	CPS	C11-C2	2.04	1.58	1.54

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	CPS	C6-C18-C17	11.98	126.61	111.81
9	A	370	CPS	C6-C18-C17	11.29	125.76	111.81
9	D	104	CPS	C6-C18-C17	11.21	125.66	111.81
9	D	103	CPS	C6-C18-C17	10.23	124.45	111.81
9	A	370	CPS	C19-C18-C17	-10.05	100.75	111.97
9	D	104	CPS	C19-C18-C17	-9.62	101.23	111.97
9	A	371	CPS	C6-C18-C17	9.15	123.12	111.81
9	D	105	CPS	C19-C18-C17	-9.06	101.85	111.97
9	D	103	CPS	C19-C18-C17	-8.89	102.04	111.97
9	A	371	CPS	C19-C18-C17	-8.80	102.15	111.97
9	D	103	CPS	C19-C3-C4	8.67	125.66	114.35
9	D	105	CPS	C19-C3-C4	8.57	125.53	114.35
9	D	104	CPS	C19-C3-C4	8.48	125.42	114.35
9	A	370	CPS	C19-C3-C4	8.38	125.29	114.35
9	A	371	CPS	C27-C26-C25	8.04	126.66	111.23
9	A	371	CPS	C19-C3-C4	7.78	124.51	114.35
9	A	370	CPS	C9-C5-C4	7.54	124.63	117.67
9	A	370	CPS	C5-C6-C18	7.54	123.36	114.81
9	D	105	CPS	C2-C19-C18	7.06	119.40	111.90
9	D	103	CPS	C2-C19-C18	6.88	119.21	111.90
9	D	104	CPS	C2-C19-C18	6.87	119.20	111.90
9	A	371	CPS	C2-C19-C18	6.58	118.89	111.90
9	A	370	CPS	C7-C6-C18	-6.54	109.00	118.30
9	A	371	CPS	C26-C27-N2	6.32	130.82	115.39
9	D	104	CPS	C9-C5-C4	6.31	123.49	117.67
9	D	103	CPS	C10-C5-C6	-6.30	101.22	111.22
9	D	104	CPS	C5-C6-C18	6.29	121.94	114.81
9	A	371	CPS	C3-C19-C18	-6.23	101.84	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	103	CPS	C5-C6-C18	6.18	121.81	114.81
9	D	103	CPS	C3-C19-C18	-6.16	101.95	110.81
9	A	370	CPS	C3-C19-C18	-6.08	102.07	110.81
9	D	103	CPS	C15-C16-C17	6.01	120.86	114.46
9	D	104	CPS	C3-C19-C18	-5.98	102.21	110.81
9	D	105	CPS	C3-C19-C18	-5.95	102.25	110.81
9	D	105	CPS	C5-C6-C18	5.94	121.55	114.81
9	D	103	CPS	C9-C5-C4	5.92	123.13	117.67
9	D	103	CPS	C7-C6-C18	-5.91	109.90	118.30
9	D	104	CPS	C7-C6-C18	-5.81	110.04	118.30
9	D	105	CPS	C10-C5-C6	-5.74	102.10	111.22
9	D	105	CPS	C15-C16-C17	5.63	120.46	114.46
9	D	104	CPS	C10-C5-C6	-5.55	102.40	111.22
9	A	370	CPS	C2-C19-C18	5.55	117.80	111.90
9	A	370	CPS	C5-C9-C20	5.53	126.17	119.51
9	D	105	CPS	C9-C5-C6	5.51	105.69	100.07
9	A	370	CPS	C10-C5-C6	-5.25	102.88	111.22
9	D	105	CPS	C7-C6-C18	-5.24	110.84	118.30
9	A	371	CPS	C10-C5-C6	-5.16	103.03	111.22
9	A	371	CPS	C6-C5-C4	5.15	112.17	107.40
9	A	371	CPS	C15-C16-C17	5.13	119.93	114.46
9	D	105	CPS	C9-C5-C4	4.91	122.20	117.67
9	A	370	CPS	C10-C5-C4	-4.90	104.19	109.08
9	A	371	CPS	C5-C6-C18	4.81	120.26	114.81
9	D	103	CPS	C7-C6-C5	4.79	108.38	103.58
9	D	104	CPS	C7-C6-C5	4.73	108.32	103.58
9	D	103	CPS	C5-C9-C20	4.72	125.19	119.51
9	A	371	CPS	C9-C5-C4	4.67	121.98	117.67
9	D	104	CPS	C9-C5-C6	4.53	104.70	100.07
9	A	371	CPS	C31-C30-N2	4.50	126.39	115.39
9	D	104	CPS	C10-C5-C4	-4.49	104.60	109.08
9	D	104	CPS	C15-C16-C17	4.42	119.17	114.46
9	A	370	CPS	C15-C16-C17	4.39	119.14	114.46
9	A	370	CPS	C7-C6-C5	4.25	107.83	103.58
9	D	103	CPS	C6-C5-C4	4.19	111.28	107.40
9	A	371	CPS	C7-C6-C18	-4.16	112.39	118.30
9	A	371	CPS	O4-C4-C5	-4.15	104.32	111.13
9	A	370	CPS	C11-C2-C19	-4.10	105.86	111.17
9	D	104	CPS	C5-C9-C20	4.06	124.39	119.51
9	A	371	CPS	C9-C5-C6	4.05	104.20	100.07
9	D	105	CPS	O4-C4-C5	-4.02	104.53	111.13
9	A	370	CPS	O4-C4-C5	-4.00	104.56	111.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	CPS	C16-C17-C18	3.97	115.71	111.51
9	D	104	CPS	C6-C5-C4	3.87	110.98	107.40
9	D	103	CPS	C9-C5-C6	3.87	104.02	100.07
9	D	105	CPS	C6-C5-C4	3.85	110.96	107.40
9	A	370	CPS	C11-C2-C1	3.80	114.64	108.17
9	D	103	CPS	C16-C17-C18	3.80	115.53	111.51
9	D	103	CPS	C10-C5-C4	-3.76	105.33	109.08
9	A	371	CPS	C16-C17-C18	3.73	115.46	111.51
9	A	370	CPS	C6-C5-C4	3.71	110.83	107.40
9	A	370	CPS	C8-C9-C20	-3.71	105.21	112.06
9	D	104	CPS	O4-C4-C5	-3.70	105.06	111.13
9	D	105	CPS	C21-C20-C9	3.65	119.35	112.96
9	D	103	CPS	C21-C20-C9	3.65	119.35	112.96
9	D	104	CPS	C16-C17-C18	3.63	115.36	111.51
9	A	370	CPS	C16-C17-C18	3.47	115.19	111.51
9	D	103	CPS	C15-C14-C13	-3.42	107.93	112.95
9	D	103	CPS	O4-C4-C5	-3.40	105.54	111.13
9	D	105	CPS	C7-C6-C5	3.38	106.97	103.58
9	A	371	CPS	C11-C2-C19	-3.37	106.81	111.17
9	A	371	CPS	C10-C5-C4	-3.29	105.80	109.08
9	D	104	CPS	C21-C20-C9	3.28	118.71	112.96
9	A	370	CPS	C9-C5-C6	3.28	103.42	100.07
9	D	103	CPS	O4-C4-C3	-3.25	102.46	108.99
9	D	105	CPS	C5-C9-C20	3.18	123.34	119.51
9	A	371	CPS	O4-C4-C3	-3.16	102.62	108.99
9	D	105	CPS	C19-C2-C15	-3.15	104.29	108.67
9	A	370	CPS	C15-C14-C13	-3.12	108.37	112.95
9	A	370	CPS	O3-C17-C18	-3.05	102.77	109.23
9	A	371	CPS	C5-C9-C20	3.04	123.17	119.51
9	D	104	CPS	C15-C14-C13	-3.02	108.52	112.95
9	A	371	CPS	C26-C25-N1	2.92	121.00	112.21
9	A	371	CPS	O3-C17-C18	-2.91	103.07	109.23
9	A	370	CPS	C21-C20-C9	2.91	118.05	112.96
9	A	371	CPS	C15-C14-C13	-2.86	108.75	112.95
9	D	105	CPS	C11-C2-C1	2.84	113.01	108.17
9	D	103	CPS	C11-C2-C1	2.83	112.99	108.17
9	D	104	CPS	O3-C17-C18	-2.80	103.30	109.23
9	D	103	CPS	C19-C2-C15	-2.76	104.83	108.67
9	D	104	CPS	C11-C2-C19	-2.76	107.60	111.17
9	D	104	CPS	C8-C9-C20	-2.75	106.99	112.06
9	D	104	CPS	C16-C15-C14	-2.73	107.89	111.14
9	D	105	CPS	C15-C14-C13	-2.73	108.94	112.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	CPS	O3-C17-C18	-2.71	103.48	109.23
9	D	104	CPS	C11-C2-C1	2.71	112.78	108.17
9	D	103	CPS	C11-C2-C19	-2.71	107.67	111.17
9	D	103	CPS	O3-C17-C18	-2.66	103.60	109.23
9	D	105	CPS	C10-C5-C9	-2.62	107.06	111.22
9	A	370	CPS	C14-C15-C2	2.62	115.50	112.67
9	D	105	CPS	O4-C4-C3	-2.61	103.74	108.99
9	D	104	CPS	O4-C4-C3	-2.61	103.75	108.99
9	D	103	CPS	C16-C15-C14	-2.61	108.04	111.14
9	D	104	CPS	C1-C12-C13	2.60	114.68	110.37
9	A	371	CPS	C16-C15-C14	-2.60	108.05	111.14
9	A	371	CPS	O1S-S-O3S	-2.57	107.47	112.44
9	D	103	CPS	C8-C9-C20	-2.47	107.49	112.06
9	D	103	CPS	C14-C15-C2	2.44	115.31	112.67
9	A	370	CPS	C1-C12-C13	2.43	114.39	110.37
9	A	370	CPS	O4-C4-C3	-2.40	104.17	108.99
9	D	103	CPS	C1-C12-C13	2.39	114.33	110.37
9	A	371	CPS	O1-C24-C23	2.39	126.67	121.92
9	D	105	CPS	C1-C12-C13	2.38	114.31	110.37
9	D	104	CPS	C19-C2-C15	-2.34	105.42	108.67
9	A	371	CPS	C21-C20-C9	2.30	116.98	112.96
9	A	371	CPS	C7-C8-C9	-2.28	100.51	105.14
9	A	371	CPS	C19-C2-C15	-2.16	105.67	108.67
9	A	370	CPS	C3-C4-C5	-2.15	109.00	111.21
9	D	105	CPS	C11-C2-C19	-2.14	108.41	111.17
9	D	104	CPS	C14-C15-C2	2.13	114.97	112.67
9	D	105	CPS	C10-C5-C4	-2.10	106.99	109.08
9	D	105	CPS	C16-C15-C14	-2.08	108.67	111.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	371	CPS	C25-C26-C27-N2

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.