



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:30 PM UTC

PDB ID : 6O7A / pdb_00006o7a
Title : Crystal structure of the LjCASTOR gating ring in the Ca²⁺-free state
Authors : Jiang, Y.; Kim, S.
Deposited on : 2019-03-07
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
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

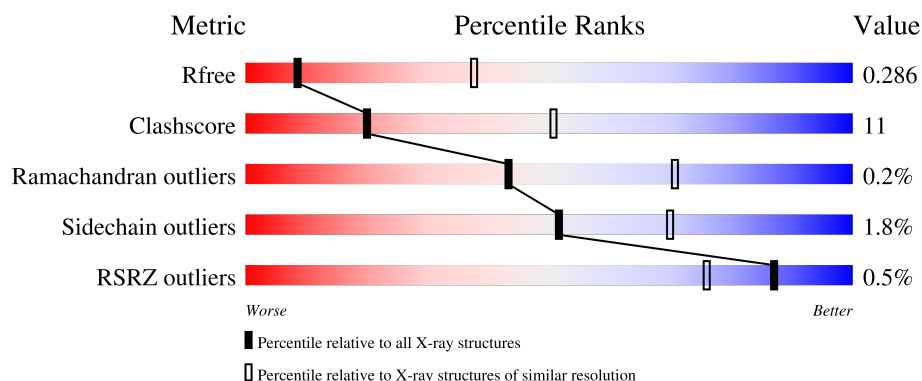
1 Overall quality at a glance

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	554	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>31%</div> <div>• 9%</div> </div> </div>
1	B	554	<div> <div>73%</div> <div>18%</div> <div>• 9%</div> </div>
1	C	554	<div> <div>66%</div> <div>25%</div> <div>9%</div> </div>
1	D	554	<div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15882 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 Ion channel CASTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3970	2504	681	764	21			
1	C	506	Total	C	N	O	S	0	0	0
			3970	2504	681	764	21			
1	B	505	Total	C	N	O	S	0	0	0
			3963	2499	680	763	21			
1	D	507	Total	C	N	O	S	0	0	0
			3979	2509	682	767	21			

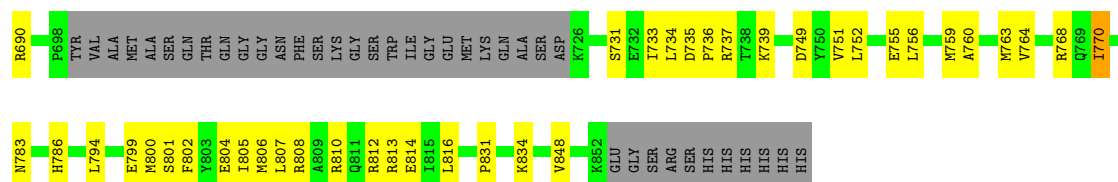
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	MET	-	expression tag	UNP Q5H8A6
A	311	ALA	-	expression tag	UNP Q5H8A6
A	854	GLY	-	expression tag	UNP Q5H8A6
A	855	SER	-	expression tag	UNP Q5H8A6
A	856	ARG	-	expression tag	UNP Q5H8A6
A	857	SER	-	expression tag	UNP Q5H8A6
A	858	HIS	-	expression tag	UNP Q5H8A6
A	859	HIS	-	expression tag	UNP Q5H8A6
A	860	HIS	-	expression tag	UNP Q5H8A6
A	861	HIS	-	expression tag	UNP Q5H8A6
A	862	HIS	-	expression tag	UNP Q5H8A6
A	863	HIS	-	expression tag	UNP Q5H8A6
C	310	MET	-	expression tag	UNP Q5H8A6
C	311	ALA	-	expression tag	UNP Q5H8A6
C	854	GLY	-	expression tag	UNP Q5H8A6
C	855	SER	-	expression tag	UNP Q5H8A6
C	856	ARG	-	expression tag	UNP Q5H8A6
C	857	SER	-	expression tag	UNP Q5H8A6
C	858	HIS	-	expression tag	UNP Q5H8A6
C	859	HIS	-	expression tag	UNP Q5H8A6
C	860	HIS	-	expression tag	UNP Q5H8A6

Continued on next page...

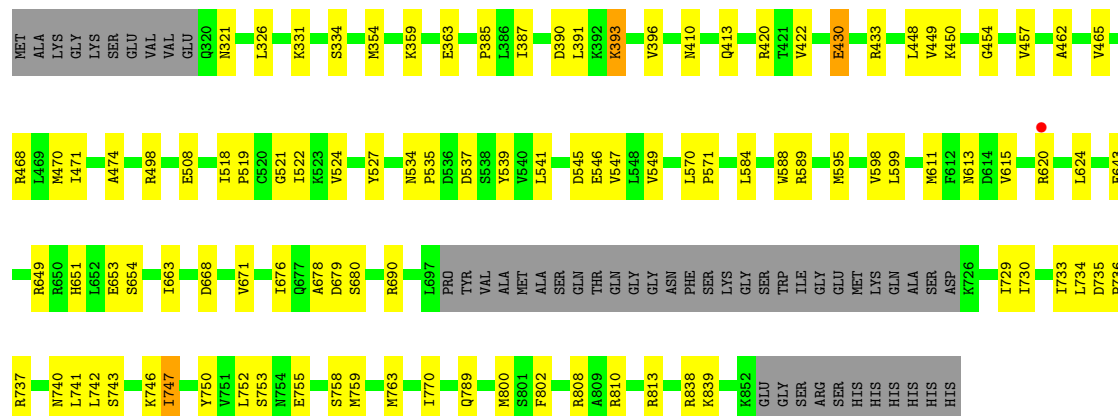
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	861	HIS	-	expression tag	UNP Q5H8A6
C	862	HIS	-	expression tag	UNP Q5H8A6
C	863	HIS	-	expression tag	UNP Q5H8A6
B	310	MET	-	expression tag	UNP Q5H8A6
B	311	ALA	-	expression tag	UNP Q5H8A6
B	854	GLY	-	expression tag	UNP Q5H8A6
B	855	SER	-	expression tag	UNP Q5H8A6
B	856	ARG	-	expression tag	UNP Q5H8A6
B	857	SER	-	expression tag	UNP Q5H8A6
B	858	HIS	-	expression tag	UNP Q5H8A6
B	859	HIS	-	expression tag	UNP Q5H8A6
B	860	HIS	-	expression tag	UNP Q5H8A6
B	861	HIS	-	expression tag	UNP Q5H8A6
B	862	HIS	-	expression tag	UNP Q5H8A6
B	863	HIS	-	expression tag	UNP Q5H8A6
D	310	MET	-	expression tag	UNP Q5H8A6
D	311	ALA	-	expression tag	UNP Q5H8A6
D	854	GLY	-	expression tag	UNP Q5H8A6
D	855	SER	-	expression tag	UNP Q5H8A6
D	856	ARG	-	expression tag	UNP Q5H8A6
D	857	SER	-	expression tag	UNP Q5H8A6
D	858	HIS	-	expression tag	UNP Q5H8A6
D	859	HIS	-	expression tag	UNP Q5H8A6
D	860	HIS	-	expression tag	UNP Q5H8A6
D	861	HIS	-	expression tag	UNP Q5H8A6
D	862	HIS	-	expression tag	UNP Q5H8A6
D	863	HIS	-	expression tag	UNP Q5H8A6



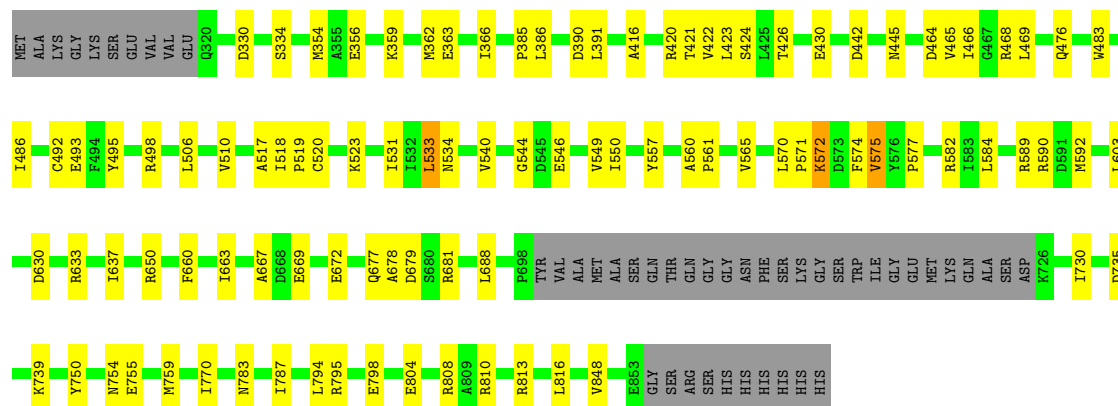
• Molecule 1: Ion channel CASTOR

Chain B: 73% 18% 9%



• Molecule 1: Ion channel CASTOR

Chain D: 74% 17% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.43Å 116.02Å 113.03Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	41.47 – 3.30 41.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.47-3.30) 94.7 (41.47-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.229 , 0.284 0.230 , 0.286	Depositor DCC
R_{free} test set	1996 reflections (5.56%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15882	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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](#)

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	0.27	0/4026	0.50	1/5440 (0.0%)
1	B	0.23	0/4018	0.45	0/5428
1	C	0.22	0/4026	0.44	0/5440
1	D	0.22	0/4035	0.43	0/5452
All	All	0.23	0/16105	0.46	1/21760 (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	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	794	LEU	CA-CB-CG	-5.22	98.04	116.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	571	PRO	Peptide
1	A	792	ILE	Peptide
1	A	843	LYS	Peptide

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	3970	0	4033	137	1
1	B	3963	0	4026	74	0
1	C	3970	0	4033	98	1
1	D	3979	0	4039	65	0
All	All	15882	0	16131	364	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (364) 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:C:805:ILE:HG23	1:C:808:ARG:HH21	1.45	0.82
1:D:589:ARG:H	1:D:592:MET:HE3	1.45	0.81
1:C:794:LEU:HB3	1:C:808:ARG:HH12	1.46	0.80
1:A:739:LYS:HD2	1:A:753:SER:HB3	1.64	0.79
1:B:800:MET:HE1	1:B:808:ARG:HE	1.48	0.79
1:B:470:MET:HG2	1:B:752:LEU:HD21	1.66	0.78
1:B:534:ASN:O	1:B:813:ARG:NH2	2.17	0.77
1:D:735:ASP:HB3	1:D:739:LYS:HZ3	1.50	0.76
1:B:611:MET:SD	1:B:620:ARG:NH2	2.59	0.76
1:A:581:GLU:HG3	1:A:603:LEU:HD11	1.68	0.75
1:A:683:LEU:HD21	1:A:733:ILE:HD11	1.68	0.74
1:C:800:MET:HE1	1:C:808:ARG:HD3	1.71	0.73
1:D:498:ARG:HH21	1:D:544:GLY:H	1.36	0.73
1:B:390:ASP:HA	1:B:393:LYS:HE3	1.71	0.72
1:A:787:ILE:HG22	1:A:847:VAL:HA	1.71	0.72
1:D:498:ARG:HB2	1:D:546:GLU:HG2	1.70	0.72
1:C:463:HIS:HE1	1:C:590:ARG:HB3	1.54	0.72
1:A:330:ASP:HB3	1:A:736:PRO:HD3	1.72	0.72
1:C:763:MET:HE2	1:C:770:ILE:HD13	1.72	0.72
1:A:629:LEU:HD11	1:A:634:LEU:HD21	1.73	0.69
1:A:736:PRO:HA	1:A:739:LYS:HD3	1.73	0.69
1:D:523:LYS:HA	1:D:531:ILE:HG22	1.73	0.69
1:A:650:ARG:HA	1:A:653:GLU:HG3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ARG:NH1	1:B:653:GLU:OE1	2.26	0.69
1:D:565:VAL:HG13	1:D:804:GLU:HG2	1.75	0.68
1:C:593:GLU:HG3	1:C:624:LEU:HD12	1.76	0.68
1:C:456:LEU:HD22	1:C:768:ARG:HH12	1.59	0.67
1:A:511:LEU:HA	1:A:519:PRO:HG2	1.77	0.67
1:A:571:PRO:HG3	1:A:795:ARG:HD3	1.76	0.67
1:B:730:ILE:HA	1:B:750:TYR:O	1.94	0.67
1:A:565:VAL:HG21	1:A:807:LEU:HD13	1.76	0.67
1:C:816:LEU:HA	1:C:848:VAL:HG12	1.76	0.66
1:A:386:LEU:HD22	1:A:420:ARG:HG3	1.78	0.66
1:D:359:LYS:NZ	1:D:363:GLU:OE2	2.29	0.66
1:A:805:ILE:HG21	1:A:846:PHE:CZ	2.31	0.66
1:B:680:SER:HB3	1:D:416:ALA:HB1	1.78	0.66
1:C:570:LEU:HD12	1:C:808:ARG:HH11	1.61	0.65
1:A:770:ILE:O	1:A:773:VAL:HG12	1.97	0.65
1:A:733:ILE:HD12	1:A:751:VAL:HG11	1.78	0.65
1:B:539:TYR:OH	1:B:545:ASP:OD2	2.14	0.65
1:A:326:LEU:HD13	1:A:385:PRO:HB3	1.78	0.64
1:D:816:LEU:HA	1:D:848:VAL:HG12	1.79	0.64
1:A:489:PHE:HE2	1:A:763:MET:HG2	1.60	0.64
1:C:800:MET:SD	1:C:808:ARG:NH1	2.70	0.64
1:D:533:LEU:HD11	1:D:783:ASN:HB2	1.79	0.63
1:C:366:ILE:HA	1:C:369:MET:HE2	1.81	0.63
1:C:410:ASN:HB3	1:C:413:GLN:HB2	1.79	0.63
1:A:565:VAL:HB	1:A:804:GLU:HG2	1.81	0.62
1:C:511:LEU:HD12	1:C:512:ILE:HG23	1.81	0.62
1:B:519:PRO:HA	1:B:549:VAL:HG12	1.80	0.62
1:A:794:LEU:HD11	1:A:846:PHE:CZ	2.35	0.62
1:A:801:SER:HB2	1:A:836:GLY:HA2	1.81	0.61
1:C:492:CYS:HA	1:C:551:ALA:O	2.00	0.61
1:B:508:GLU:HB3	1:B:537:ASP:HB3	1.81	0.61
1:A:498:ARG:HB2	1:A:546:GLU:HG2	1.82	0.61
1:A:584:LEU:HD12	1:A:663:ILE:HG23	1.82	0.61
1:C:462:ALA:O	1:C:465:VAL:HG12	2.01	0.61
1:B:410:ASN:HB3	1:B:413:GLN:HB2	1.82	0.61
1:B:422:VAL:HG21	1:B:449:VAL:HG13	1.84	0.60
1:C:435:HIS:HB3	1:C:768:ARG:HH11	1.65	0.60
1:C:336:LEU:HD12	1:C:369:MET:HE1	1.82	0.60
1:B:736:PRO:HG3	1:B:755:GLU:HG3	1.83	0.59
1:C:585:PHE:HE1	1:C:664:LEU:HD12	1.68	0.59
1:A:571:PRO:HG2	1:A:792:ILE:HG22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:MET:HE3	1:A:380:CYS:HB3	1.85	0.59
1:C:812:ARG:HB3	1:C:814:GLU:HG3	1.85	0.58
1:A:588:TRP:NE1	1:A:669:GLU:OE2	2.31	0.58
1:A:511:LEU:HD12	1:A:512:ILE:HG23	1.85	0.58
1:A:639:LEU:HD23	1:A:639:LEU:H	1.69	0.58
1:C:487:LEU:HD12	1:C:756:LEU:HD12	1.85	0.58
1:A:590:ARG:HA	1:A:669:GLU:HG2	1.85	0.58
1:C:570:LEU:HB2	1:C:808:ARG:HD2	1.86	0.58
1:A:834:LYS:HD3	1:A:837:ARG:HD3	1.85	0.57
1:A:514:PHE:O	1:A:803:TYR:OH	2.22	0.57
1:B:741:LEU:HB3	1:D:423:LEU:HG	1.86	0.57
1:A:420:ARG:HD3	1:D:739:LYS:HE3	1.87	0.57
1:A:534:ASN:HA	1:A:815:ILE:HD11	1.86	0.57
1:C:539:TYR:OH	1:C:545:ASP:OD2	2.21	0.57
1:A:531:ILE:HD11	1:A:769:GLN:HB3	1.86	0.57
1:A:829:ILE:HG23	1:A:830:ASN:OD1	2.05	0.57
1:A:837:ARG:HE	1:A:838:ARG:H	1.53	0.57
1:A:518:ILE:HB	1:A:830:ASN:ND2	2.20	0.56
1:A:432:LEU:HD12	1:A:456:LEU:HD13	1.87	0.56
1:A:373:PHE:HB3	1:A:376:THR:HB	1.87	0.56
1:A:622:LYS:HA	1:A:625:ILE:HG22	1.88	0.56
1:A:649:ARG:HH21	1:A:692:ILE:HD11	1.69	0.56
1:B:620:ARG:NH2	1:B:624:LEU:HD11	2.21	0.56
1:A:787:ILE:O	1:A:788:ARG:HG2	2.06	0.56
1:A:675:ALA:HB1	1:A:735:ASP:OD2	2.05	0.56
1:C:620:ARG:HH22	1:C:642:ARG:C	2.14	0.56
1:A:514:PHE:HE2	1:A:559:PRO:HB3	1.70	0.56
1:A:381:ARG:HH11	1:A:393:LYS:HE2	1.70	0.55
1:D:735:ASP:O	1:D:739:LYS:HG2	2.07	0.55
1:D:590:ARG:HH21	1:D:672:GLU:HG2	1.71	0.55
1:A:579:SER:HB3	1:A:603:LEU:HD22	1.88	0.55
1:C:605:PRO:HA	1:C:636:ASN:HB3	1.87	0.54
1:B:741:LEU:HD22	1:D:424:SER:HA	1.87	0.54
1:A:588:TRP:HZ2	1:A:623:LYS:HD2	1.72	0.54
1:D:755:GLU:HG2	1:D:759:MET:HE3	1.90	0.54
1:A:581:GLU:CG	1:A:603:LEU:HD11	2.37	0.54
1:A:830:ASN:OD1	1:A:830:ASN:N	2.40	0.54
1:C:385:PRO:HB2	1:C:421:THR:HG23	1.90	0.54
1:C:567:ARG:HD3	1:C:807:LEU:HD13	1.90	0.54
1:D:386:LEU:HD22	1:D:420:ARG:HG3	1.90	0.54
1:C:470:MET:HE2	1:C:664:LEU:HD22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:ASN:HD22	1:D:783:ASN:ND2	2.06	0.54
1:C:596:ILE:HD12	1:C:624:LEU:HD11	1.90	0.53
1:C:474:ALA:HB2	1:C:664:LEU:HD21	1.89	0.53
1:B:450:LYS:O	1:B:454:GLY:N	2.29	0.53
1:D:523:LYS:HB3	1:D:546:GLU:HB2	1.89	0.53
1:A:541:LEU:HB3	1:A:545:ASP:OD2	2.08	0.53
1:A:814:GLU:HB3	1:A:848:VAL:HG11	1.91	0.53
1:C:794:LEU:HD23	1:C:808:ARG:HH22	1.73	0.53
1:A:441:SER:O	1:A:590:ARG:NH2	2.31	0.53
1:D:466:ILE:HD11	1:D:754:ASN:HA	1.91	0.53
1:C:620:ARG:NH2	1:C:642:ARG:O	2.38	0.53
1:B:800:MET:HE1	1:B:808:ARG:NE	2.19	0.53
1:D:334:SER:OG	1:D:755:GLU:HG3	2.08	0.53
1:D:603:LEU:HB2	1:D:637:ILE:HD11	1.91	0.53
1:B:354:MET:SD	1:B:390:ASP:HB3	2.48	0.53
1:C:497:LYS:HD3	1:C:499:TRP:CZ2	2.44	0.53
1:C:805:ILE:HG23	1:C:808:ARG:NH2	2.21	0.52
1:D:575:VAL:O	1:D:577:PRO:HD3	2.08	0.52
1:A:511:LEU:HD13	1:A:806:MET:HE2	1.91	0.52
1:B:740:ASN:O	1:B:743:SER:OG	2.26	0.52
1:C:565:VAL:HG13	1:C:804:GLU:HG2	1.92	0.52
1:D:430:GLU:OE1	1:D:430:GLU:N	2.43	0.52
1:C:368:LYS:HB3	1:B:387:ILE:HG21	1.92	0.51
1:C:687:LEU:HB3	1:B:448:LEU:HD22	1.92	0.51
1:C:755:GLU:HB3	1:C:759:MET:HE3	1.93	0.51
1:A:805:ILE:HG21	1:A:846:PHE:CE1	2.45	0.51
1:A:620:ARG:HA	1:A:623:LYS:HG3	1.93	0.51
1:C:493:GLU:OE1	1:C:493:GLU:N	2.41	0.51
1:A:800:MET:HE1	1:A:808:ARG:HD2	1.92	0.51
1:C:506:LEU:O	1:C:510:VAL:HG23	2.11	0.51
1:B:838:ARG:NH1	1:B:839:LYS:O	2.44	0.51
1:A:726:LYS:HD2	1:A:747:ILE:HG21	1.92	0.51
1:A:585:PHE:HE2	1:A:609:LEU:HG	1.75	0.51
1:C:586:CYS:HB2	1:C:665:ILE:HA	1.92	0.51
1:A:579:SER:HB3	1:A:603:LEU:HD13	1.93	0.51
1:A:619:GLU:OE2	1:A:623:LYS:HE2	2.12	0.50
1:A:474:ALA:HB2	1:A:664:LEU:HD21	1.93	0.50
1:B:651:HIS:O	1:B:654:SER:OG	2.17	0.50
1:D:506:LEU:HD23	1:D:540:VAL:HG22	1.94	0.50
1:D:798:GLU:OE2	1:D:808:ARG:NH2	2.43	0.50
1:B:471:ILE:HD13	1:B:599:LEU:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:PRO:HB2	1:D:421:THR:HG23	1.93	0.50
1:A:763:MET:HE2	1:A:770:ILE:HG21	1.93	0.50
1:D:534:ASN:O	1:D:813:ARG:NH2	2.44	0.50
1:D:667:ALA:HB1	1:D:678:ALA:HB1	1.94	0.50
1:C:423:LEU:O	1:C:426:THR:OG1	2.25	0.50
1:C:794:LEU:HB3	1:C:808:ARG:NH1	2.22	0.50
1:B:570:LEU:HB2	1:B:808:ARG:HH12	1.76	0.50
1:B:649:ARG:O	1:B:653:GLU:HG3	2.12	0.50
1:A:834:LYS:HB3	1:A:837:ARG:HG2	1.94	0.49
1:B:735:ASP:OD1	1:B:737:ARG:HB3	2.12	0.49
1:B:690:ARG:CZ	1:B:729:ILE:HD12	2.42	0.49
1:B:742:LEU:HD11	1:B:746:LYS:CB	2.43	0.49
1:D:506:LEU:O	1:D:510:VAL:HG23	2.12	0.49
1:A:464:ASP:OD2	1:A:468:ARG:NH2	2.42	0.49
1:A:570:LEU:O	1:A:572:LYS:HG3	2.12	0.49
1:A:629:LEU:HD21	1:A:634:LEU:HD11	1.95	0.49
1:A:733:ILE:HD13	1:A:738:THR:HG22	1.95	0.49
1:D:572:LYS:HD3	1:D:574:PHE:CZ	2.47	0.49
1:A:671:VAL:O	1:A:678:ALA:HB2	2.12	0.49
1:B:331:LYS:HB3	1:B:758:SER:OG	2.12	0.49
1:C:466:ILE:CG2	1:C:589:ARG:HH12	2.26	0.49
1:C:511:LEU:HA	1:C:519:PRO:HG2	1.93	0.49
1:A:739:LYS:HZ1	1:A:755:GLU:HB2	1.77	0.48
1:C:676:ILE:HA	1:C:735:ASP:OD2	2.12	0.48
1:B:449:VAL:HG12	1:B:457:VAL:HG11	1.94	0.48
1:C:527:TYR:HB3	1:C:530:LYS:HE3	1.96	0.48
1:A:816:LEU:HG	1:A:848:VAL:HG22	1.94	0.48
1:A:506:LEU:O	1:A:510:VAL:HG23	2.14	0.48
1:A:514:PHE:CD2	1:A:558:ALA:HB1	2.49	0.48
1:A:590:ARG:HA	1:A:669:GLU:CG	2.43	0.48
1:C:736:PRO:O	1:C:739:LYS:HB3	2.14	0.48
1:C:737:ARG:CZ	1:B:420:ARG:HD3	2.44	0.48
1:D:630:ASP:HB3	1:D:633:ARG:HD2	1.96	0.47
1:C:466:ILE:HG21	1:C:589:ARG:HH12	1.79	0.47
1:A:472:GLN:HB3	1:A:479:LEU:HD23	1.96	0.47
1:A:551:ALA:HB1	1:A:556:THR:HG21	1.95	0.47
1:A:799:GLU:HA	1:A:840:TRP:HE1	1.79	0.47
1:C:749:ASP:O	1:C:751:VAL:HG22	2.14	0.47
1:A:514:PHE:CE2	1:A:559:PRO:HB3	2.49	0.47
1:C:476:GLN:HE22	1:C:786:HIS:CD2	2.32	0.47
1:D:498:ARG:NH2	1:D:544:GLY:H	2.10	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:GLU:HG3	1:C:768:ARG:HG3	1.97	0.47
1:C:802:PHE:HB3	1:C:834:LYS:HA	1.97	0.47
1:A:582:ARG:HG3	1:A:608:GLU:HB2	1.97	0.47
1:B:391:LEU:HB3	1:B:396:VAL:HG11	1.97	0.47
1:A:585:PHE:HZ	1:A:599:LEU:HD13	1.80	0.46
1:C:582:ARG:O	1:C:661:ASP:N	2.48	0.46
1:B:733:ILE:O	1:B:753:SER:HA	2.14	0.46
1:A:816:LEU:HD12	1:A:848:VAL:HG13	1.97	0.46
1:C:731:SER:OG	1:C:751:VAL:HG11	2.16	0.46
1:A:521:GLY:HA3	1:A:548:LEU:HD23	1.98	0.46
1:C:533:LEU:HD23	1:C:783:ASN:HB2	1.98	0.46
1:A:555:ASP:OD1	1:A:555:ASP:N	2.48	0.46
1:C:446:GLU:OE2	1:C:450:LYS:HD2	2.14	0.46
1:A:739:LYS:NZ	1:A:755:GLU:HB2	2.30	0.46
1:B:522:ILE:HG12	1:B:535:PRO:HG3	1.98	0.46
1:B:539:TYR:HE2	1:B:541:LEU:HA	1.80	0.46
1:B:584:LEU:HD23	1:B:663:ILE:HG23	1.96	0.46
1:B:733:ILE:HG13	1:B:753:SER:HB3	1.97	0.46
1:A:365:ASP:OD1	1:A:365:ASP:N	2.48	0.46
1:A:523:LYS:HG2	1:A:531:ILE:HG12	1.98	0.46
1:B:498:ARG:HB2	1:B:546:GLU:HG2	1.98	0.46
1:C:466:ILE:HG22	1:C:589:ARG:HH22	1.79	0.46
1:A:506:LEU:HD12	1:A:538:SER:HA	1.97	0.46
1:A:337:ASN:HB2	1:A:371:PHE:CE1	2.51	0.46
1:B:321:ASN:HB3	1:B:433:ARG:HH11	1.81	0.46
1:D:549:VAL:HG11	1:D:557:TYR:CE2	2.51	0.46
1:A:518:ILE:HB	1:A:830:ASN:HD22	1.80	0.45
1:D:571:PRO:HG3	1:D:794:LEU:N	2.30	0.45
1:C:731:SER:H	1:C:751:VAL:HG12	1.80	0.45
1:B:524:VAL:HB	1:B:527:TYR:HB2	1.98	0.45
1:D:483:TRP:HA	1:D:486:ILE:HG22	1.98	0.45
1:D:679:ASP:CG	1:D:739:LYS:HE2	2.41	0.45
1:A:334:SER:HB2	1:A:755:GLU:HG3	1.98	0.45
1:A:324:LEU:HD12	1:A:352:ALA:O	2.17	0.45
1:A:468:ARG:HG3	1:A:598:VAL:HG11	1.98	0.45
1:A:514:PHE:HB2	1:A:519:PRO:HD3	1.99	0.45
1:C:362:MET:O	1:C:366:ILE:HG12	2.16	0.45
1:C:511:LEU:HD13	1:C:806:MET:SD	2.56	0.45
1:D:469:LEU:HD11	1:D:483:TRP:CD1	2.52	0.45
1:A:585:PHE:HZ	1:A:599:LEU:CD1	2.30	0.45
1:A:744:MET:SD	1:A:749:ASP:HB3	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:GLN:HB3	1:A:793:TYR:OH	2.16	0.45
1:D:570:LEU:HD23	1:D:570:LEU:HA	1.82	0.45
1:C:731:SER:O	1:C:751:VAL:HB	2.16	0.45
1:C:801:SER:O	1:C:805:ILE:HG13	2.16	0.45
1:D:590:ARG:HG3	1:D:669:GLU:HB2	1.98	0.45
1:C:523:LYS:HB2	1:C:531:ILE:HG12	1.97	0.45
1:C:584:LEU:HD23	1:C:663:ILE:HG23	1.99	0.45
1:A:522:ILE:CG2	1:A:541:LEU:HD21	2.47	0.45
1:B:321:ASN:OD1	1:B:321:ASN:N	2.46	0.45
1:A:733:ILE:HB	1:A:751:VAL:CG1	2.47	0.44
1:D:520:CYS:SG	1:D:550:ILE:HG13	2.57	0.44
1:A:468:ARG:HD3	1:A:779:ALA:HA	1.99	0.44
1:B:588:TRP:O	1:B:668:ASP:HA	2.17	0.44
1:D:730:ILE:HG23	1:D:750:TYR:O	2.17	0.44
1:A:501:GLN:N	1:A:501:GLN:OE1	2.50	0.44
1:B:521:GLY:HA2	1:B:535:PRO:HD3	2.00	0.44
1:B:613:ASN:HD22	1:B:615:VAL:HB	1.83	0.44
1:B:789:GLN:H	1:B:789:GLN:HG2	1.60	0.44
1:A:837:ARG:HD2	1:A:837:ARG:HA	1.72	0.44
1:C:600:ASP:OD1	1:C:637:ILE:HD12	2.17	0.44
1:C:613:ASN:O	1:C:643:GLU:HA	2.16	0.44
1:A:453:GLY:HA3	1:A:457:VAL:HG21	2.00	0.44
1:A:482:ILE:HG23	1:A:829:ILE:HD11	1.99	0.44
1:A:506:LEU:HA	1:A:540:VAL:HG12	2.00	0.44
1:A:522:ILE:HD12	1:A:535:PRO:HG3	2.00	0.44
1:B:810:ARG:HA	1:B:810:ARG:HD2	1.73	0.44
1:B:539:TYR:CE2	1:B:541:LEU:HA	2.52	0.44
1:A:493:GLU:OE2	1:A:495:TYR:OH	2.25	0.44
1:A:784:GLU:OE2	1:A:852:LYS:HB2	2.16	0.44
1:D:510:VAL:O	1:D:519:PRO:HG2	2.18	0.44
1:A:371:PHE:CE1	1:A:373:PHE:HE1	2.36	0.44
1:A:609:LEU:HD13	1:A:637:ILE:HD12	1.99	0.44
1:D:589:ARG:N	1:D:592:MET:HE3	2.22	0.44
1:D:810:ARG:HD2	1:D:810:ARG:HA	1.73	0.44
1:B:679:ASP:CG	1:B:734:LEU:H	2.25	0.44
1:D:354:MET:SD	1:D:390:ASP:HB3	2.58	0.44
1:C:534:ASN:ND2	1:C:813:ARG:O	2.30	0.43
1:C:735:ASP:HB3	1:C:737:ARG:H	1.83	0.43
1:B:611:MET:HB3	1:B:611:MET:HE2	1.80	0.43
1:A:679:ASP:OD1	1:A:733:ILE:HG12	2.18	0.43
1:A:788:ARG:HG3	1:A:788:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:ALA:O	1:C:764:VAL:HG23	2.18	0.43
1:A:349:GLY:N	1:A:375:GLY:O	2.50	0.43
1:B:690:ARG:HD3	1:B:690:ARG:HA	1.85	0.43
1:D:571:PRO:HB2	1:D:572:LYS:HG2	2.01	0.43
1:D:582:ARG:HG2	1:D:660:PHE:HD1	1.82	0.43
1:A:588:TRP:CZ2	1:A:623:LYS:HD2	2.52	0.43
1:C:419:LEU:HD11	1:C:452:VAL:HG21	2.00	0.43
1:D:464:ASP:O	1:D:468:ARG:HG3	2.18	0.43
1:A:385:PRO:HB2	1:A:421:THR:HG22	2.01	0.43
1:B:570:LEU:N	1:B:571:PRO:CD	2.81	0.43
1:A:440:MET:HE2	1:A:440:MET:HB3	1.85	0.43
1:C:768:ARG:O	1:C:770:ILE:N	2.52	0.43
1:A:626:ASP:O	1:D:650:ARG:HB3	2.19	0.43
1:A:668:ASP:O	1:A:672:GLU:HB2	2.19	0.43
1:A:734:LEU:O	1:A:754:ASN:ND2	2.52	0.43
1:C:806:MET:O	1:C:810:ARG:HG2	2.18	0.43
1:B:518:ILE:HD11	1:B:802:PHE:HE2	1.84	0.43
1:B:755:GLU:OE1	1:B:759:MET:HE3	2.19	0.43
1:D:584:LEU:HD23	1:D:663:ILE:HG23	1.99	0.43
1:D:770:ILE:HD12	1:D:770:ILE:HA	1.84	0.43
1:C:631:ILE:O	1:C:634:LEU:HD23	2.19	0.43
1:C:687:LEU:HA	1:C:690:ARG:HG2	1.99	0.43
1:B:589:ARG:HD3	1:B:595:MET:SD	2.59	0.43
1:A:592:MET:HE2	1:A:611:MET:SD	2.59	0.43
1:D:518:ILE:C	1:D:549:VAL:HG23	2.44	0.43
1:A:785:MET:HB2	1:A:785:MET:HE3	1.70	0.42
1:C:422:VAL:O	1:C:426:THR:HG23	2.19	0.42
1:D:517:ALA:HB1	1:D:549:VAL:CG2	2.48	0.42
1:A:806:MET:HG2	1:A:816:LEU:HB2	2.01	0.42
1:C:343:ASN:HB3	1:C:348:GLY:O	2.20	0.42
1:B:747:ILE:HG22	1:B:747:ILE:O	2.19	0.42
1:B:359:LYS:O	1:B:363:GLU:HG3	2.19	0.42
1:B:671:VAL:O	1:B:678:ALA:HB2	2.18	0.42
1:A:668:ASP:OD1	1:A:668:ASP:N	2.44	0.42
1:C:391:LEU:HD22	1:C:396:VAL:HG21	2.01	0.42
1:D:442:ASP:HB3	1:D:445:ASN:OD1	2.19	0.42
1:A:794:LEU:CD2	1:A:840:TRP:HH2	2.32	0.42
1:C:461:VAL:HG22	1:C:464:ASP:HB3	2.01	0.42
1:C:802:PHE:CE1	1:C:831:PRO:HG2	2.54	0.42
1:A:520:CYS:HB3	1:A:815:ILE:HG21	2.02	0.42
1:C:440:MET:SD	1:C:449:VAL:HG21	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:ASN:O	1:C:620:ARG:NH2	2.52	0.42
1:B:321:ASN:HB3	1:B:433:ARG:NH1	2.35	0.42
1:B:742:LEU:HD11	1:B:746:LYS:HB3	2.01	0.42
1:B:326:LEU:HD13	1:B:385:PRO:HB3	2.02	0.42
1:B:462:ALA:HA	1:B:465:VAL:HG22	2.01	0.42
1:B:742:LEU:HD11	1:B:746:LYS:HB2	2.01	0.42
1:D:677:GLN:O	1:D:681:ARG:HG3	2.20	0.42
1:A:840:TRP:CD1	1:A:840:TRP:N	2.86	0.42
1:D:362:MET:O	1:D:366:ILE:HG12	2.20	0.42
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.72	0.42
1:A:814:GLU:HB3	1:A:848:VAL:CG1	2.49	0.42
1:C:359:LYS:HE2	1:C:363:GLU:OE2	2.19	0.42
1:D:422:VAL:O	1:D:426:THR:HG23	2.18	0.42
1:C:480:ALA:O	1:C:484:GLU:HG3	2.20	0.42
1:D:330:ASP:OD2	1:D:330:ASP:N	2.50	0.42
1:D:385:PRO:HA	1:D:391:LEU:HD21	2.02	0.42
1:C:400:ARG:O	1:C:434:GLY:HA3	2.20	0.41
1:D:560:ALA:HB1	1:D:561:PRO:HD2	2.02	0.41
1:C:616:PRO:O	1:C:620:ARG:HG3	2.19	0.41
1:A:649:ARG:HH21	1:A:692:ILE:CD1	2.32	0.41
1:C:583:ILE:HG23	1:C:662:SER:OG	2.20	0.41
1:B:334:SER:CB	1:B:755:GLU:HG2	2.49	0.41
1:B:613:ASN:O	1:B:643:GLU:HA	2.21	0.41
1:C:737:ARG:NH2	1:B:420:ARG:HD3	2.35	0.41
1:D:493:GLU:HB2	1:D:495:TYR:CE2	2.55	0.41
1:A:436:ILE:N	1:A:456:LEU:O	2.52	0.41
1:C:683:LEU:HD22	1:C:737:ARG:HD3	2.03	0.41
1:B:468:ARG:HG2	1:B:598:VAL:HG21	2.02	0.41
1:B:474:ALA:N	1:B:730:ILE:HD11	2.36	0.41
1:B:570:LEU:H	1:B:808:ARG:NH1	2.19	0.41
1:A:519:PRO:HB3	1:A:549:VAL:HG12	2.02	0.41
1:C:324:LEU:CD2	1:C:396:VAL:HG22	2.51	0.41
1:C:733:ILE:HD13	1:C:751:VAL:HG23	2.02	0.41
1:A:585:PHE:HE2	1:A:609:LEU:CG	2.34	0.41
1:A:814:GLU:HG2	1:A:850:THR:HB	2.02	0.41
1:C:496:ILE:HA	1:C:547:VAL:O	2.21	0.41
1:C:588:TRP:HB2	1:C:613:ASN:HB3	2.03	0.41
1:A:613:ASN:HB3	1:A:615:VAL:HG12	2.03	0.41
1:A:448:LEU:HD21	1:D:688:LEU:HD23	2.03	0.40
1:D:476:GLN:HB2	1:D:787:ILE:HB	2.03	0.40
1:A:331:LYS:HB3	1:A:758:SER:OG	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ARG:HH12	1:C:642:ARG:H	1.67	0.40
1:B:430:GLU:CD	1:B:430:GLU:H	2.30	0.40
1:A:357:ARG:NH1	1:A:362:MET:HG2	2.36	0.40
1:A:610:TRP:CD1	1:A:660:PHE:HE1	2.39	0.40
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.96	0.40
1:A:802:PHE:O	1:A:806:MET:HG3	2.22	0.40
1:C:473:CYS:HB2	1:C:752:LEU:HD21	2.04	0.40
1:C:588:TRP:O	1:C:669:GLU:N	2.42	0.40
1:C:733:ILE:O	1:C:734:LEU:HD23	2.21	0.40
1:B:620:ARG:CZ	1:B:624:LEU:HD11	2.51	0.40
1:C:808:ARG:HE	1:C:808:ARG:HB2	1.62	0.40
1:B:763:MET:HE2	1:B:770:ILE:HG21	2.03	0.40
1:D:571:PRO:HA	1:D:795:ARG:CZ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TYR:OH	1:C:799:GLU:O[1_554]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/554 (91%)	475 (95%)	23 (5%)	4 (1%)	16	45
1	B	501/554 (90%)	493 (98%)	7 (1%)	1 (0%)	43	71
1	C	502/554 (91%)	490 (98%)	12 (2%)	0	100	100
1	D	503/554 (91%)	493 (98%)	10 (2%)	0	100	100
All	All	2008/2216 (91%)	1951 (97%)	52 (3%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	PRO
1	B	747	ILE
1	A	580	PRO
1	A	671	VAL
1	A	577	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	438/476 (92%)	421 (96%)	17 (4%)	28	56
1	B	437/476 (92%)	433 (99%)	4 (1%)	70	78
1	C	438/476 (92%)	434 (99%)	4 (1%)	70	78
1	D	439/476 (92%)	433 (99%)	6 (1%)	59	73
All	All	1752/1904 (92%)	1721 (98%)	31 (2%)	51	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	A	452	VAL
1	A	465	VAL
1	A	466	ILE
1	A	470	MET
1	A	593	GLU
1	A	603	LEU
1	A	617	GLU
1	A	640	VAL
1	A	679	ASP
1	A	788	ARG
1	A	792	ILE
1	A	825	GLU
1	A	829	ILE
1	A	830	ASN
1	A	842	LEU
1	A	850	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	350	THR
1	C	457	VAL
1	C	637	ILE
1	C	770	ILE
1	B	393	LYS
1	B	430	GLU
1	B	547	VAL
1	B	676	ILE
1	D	356	GLU
1	D	465	VAL
1	D	492	CYS
1	D	533	LEU
1	D	572	LYS
1	D	575	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	789	GLN
1	C	693	GLN
1	C	786	HIS
1	B	491	ASN
1	B	783	ASN
1	D	613	ASN
1	D	693	GLN
1	D	786	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

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	506/554 (91%)	-0.02	9 (1%) 67 49	55, 117, 196, 232	0
1	B	505/554 (91%)	-0.44	1 (0%) 91 86	46, 95, 147, 202	0
1	C	506/554 (91%)	-0.26	1 (0%) 91 86	54, 122, 165, 197	0
1	D	507/554 (91%)	-0.41	0 100 100	58, 104, 148, 212	0
All	All	2024/2216 (91%)	-0.28	11 (0%) 87 76	46, 108, 172, 232	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	ALA	2.9
1	B	620	ARG	2.8
1	A	611	MET	2.8
1	A	583	ILE	2.6
1	A	793	TYR	2.6
1	A	609	LEU	2.6
1	A	602	SER	2.4
1	A	731	SER	2.3
1	A	596	ILE	2.2
1	C	679	ASP	2.2
1	A	519	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.