Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:09 AM GMT

PDB ID	:	2W2D
Title	:	Crystal Structure of a Catalytically Active, Non-toxic Endopeptidase Derivative of Clostridium botulinum Toxin A
Authors	:	Masuyer, G.; Thiyagarajan, N.; James, P.L.; Marks, P.M.H.; Chaddock, J.A.; Acharya, K.R.
Deposited on	:	2008-10-29
Resolution	:	2.59 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

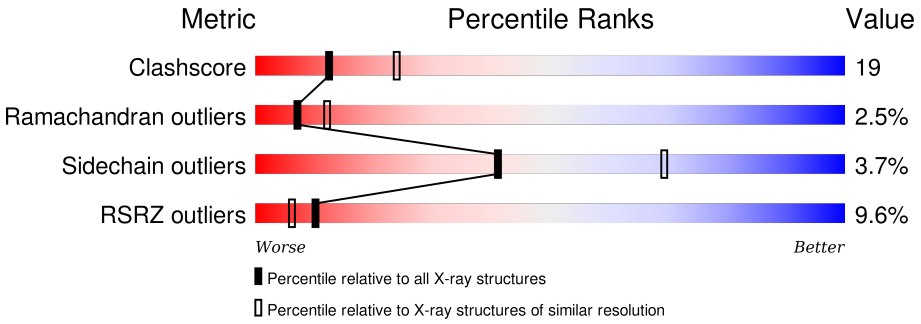
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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 <=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	450	3% 74% 21%
1	C	450	2% 75% 21%
2	B	431	12% 65% 29%
2	D	431	21% 51% 36% 6% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1433	-	-	-	X
6	GOL	A	1436	-	X	-	-
6	GOL	A	1437	-	X	-	X
6	GOL	A	1438	-	X	-	-
6	GOL	B	1873	-	X	-	-
6	GOL	B	1874	-	X	-	X
7	ACT	C	1435	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14160 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 BOTULINUM NEUROTOXIN A LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	1
			3534	2281	574	669	10			
1	C	436	Total	C	N	O	S	0	0	1
			3522	2273	573	666	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	PRO	CONFLICT	UNP A5HZZ9
A	432	ASP	ARG	CONFLICT	UNP A5HZZ9
C	2	GLU	PRO	CONFLICT	UNP A5HZZ9
C	432	ASP	ARG	CONFLICT	UNP A5HZZ9

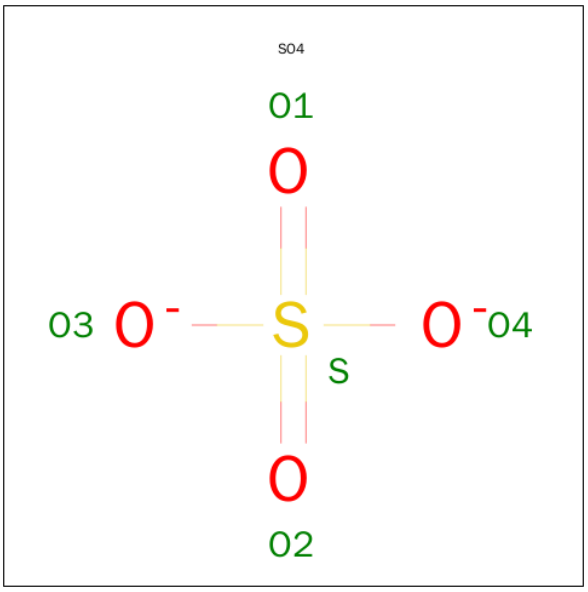
- Molecule 2 is a protein called BOTULINUM NEUROTOXIN A HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3429	2195	550	674	10			
2	D	408	Total	C	N	O	S	0	0	1
			3308	2119	529	650	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	452	LEU	ASP	CONFLICT	UNP A5HZZ9
B	453	GLN	LEU	CONFLICT	UNP A5HZZ9
D	452	LEU	ASP	CONFLICT	UNP A5HZZ9
D	453	GLN	LEU	CONFLICT	UNP A5HZZ9

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

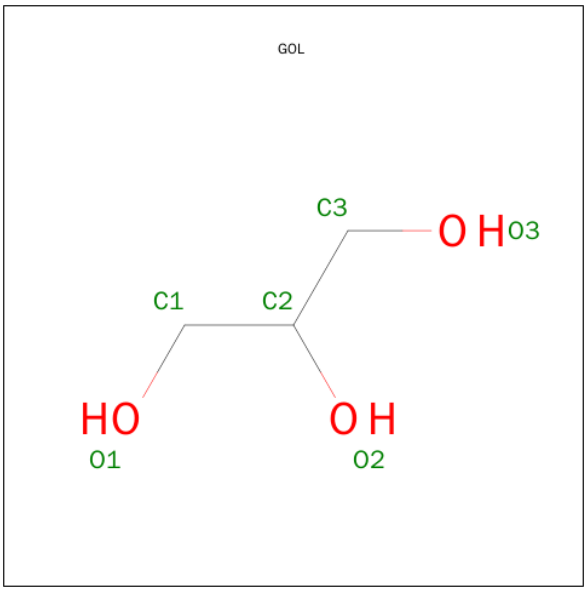
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

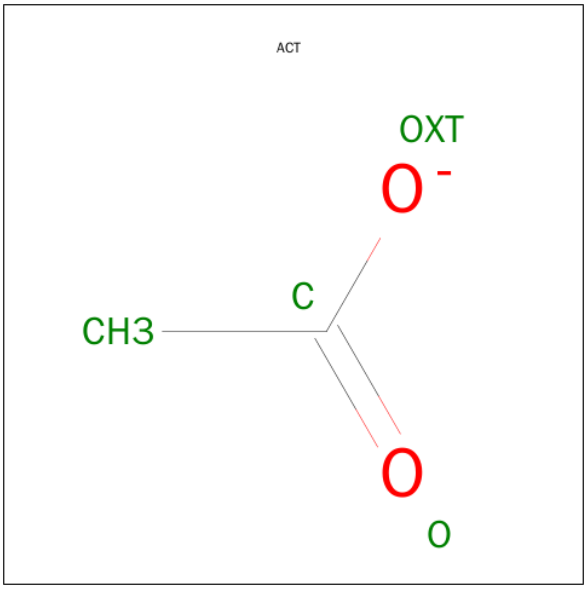
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

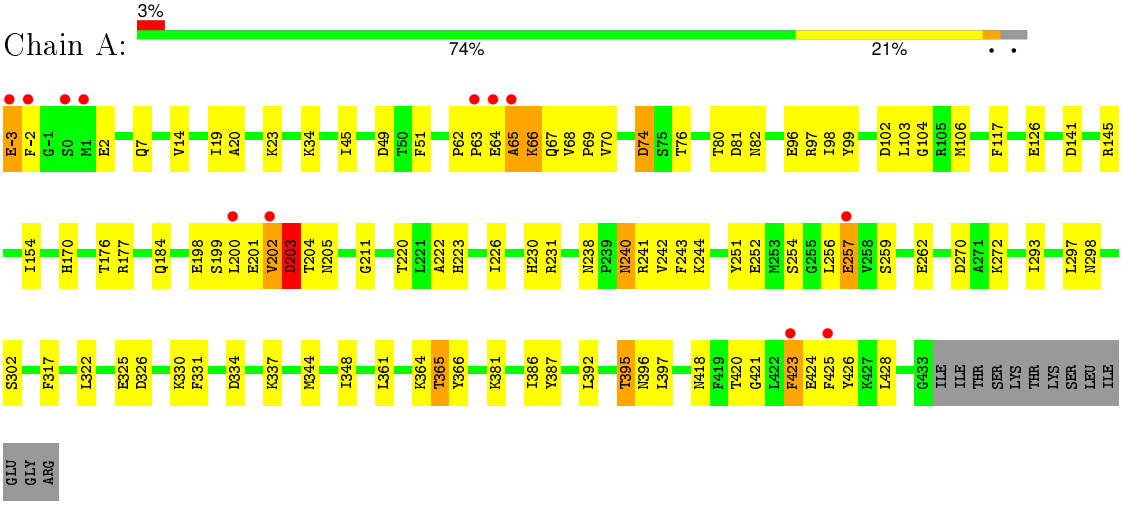
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	49	Total O 49 49	0	0
8	C	118	Total O 118 118	0	0
8	D	31	Total O 31 31	0	0

3 Residue-property plots (i)

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.

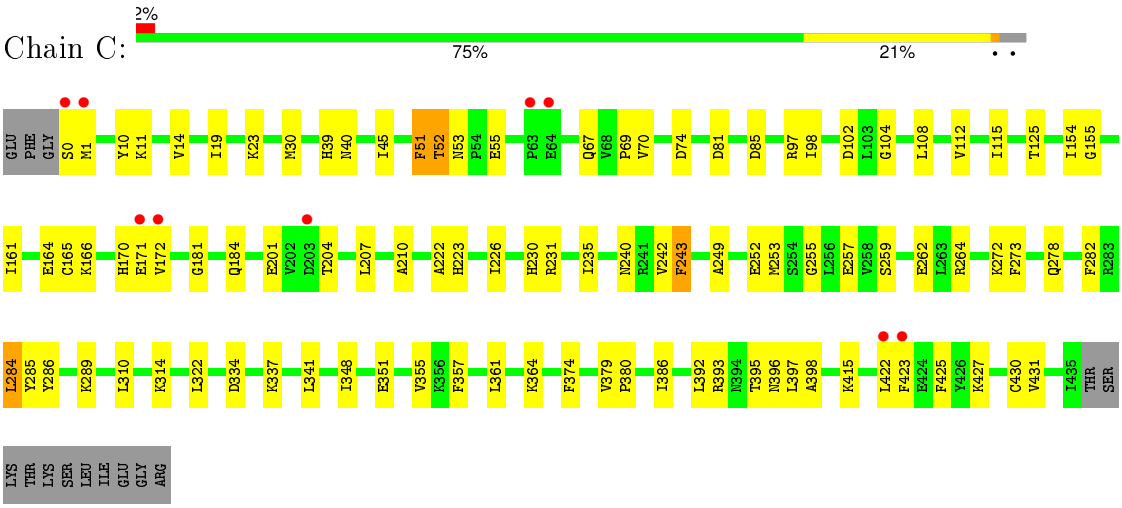
- Molecule 1: BOTULINUM NEUROTOXIN A LIGHT CHAIN

Chain A:



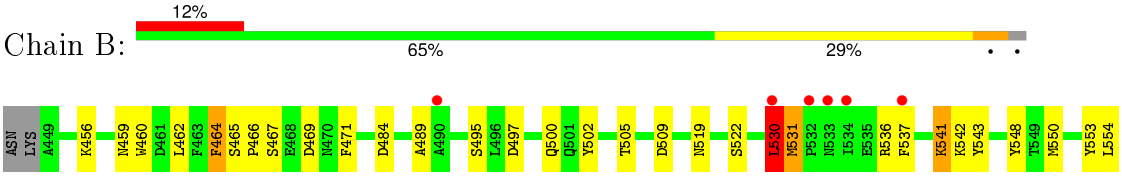
- Molecule 1: BOTULINUM NEUROTOXIN A LIGHT CHAIN

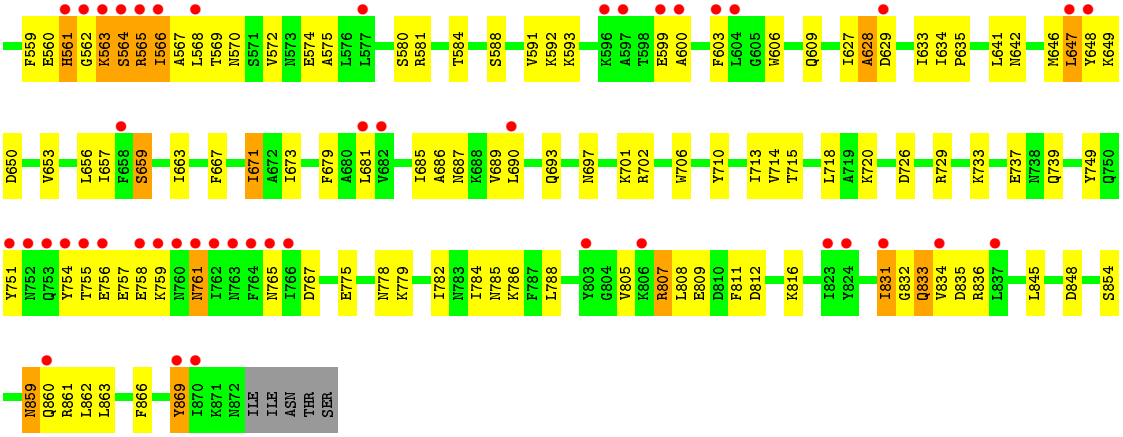
Chain C:



- Molecule 2: BOTULINUM NEUROTOXIN A HEAVY CHAIN

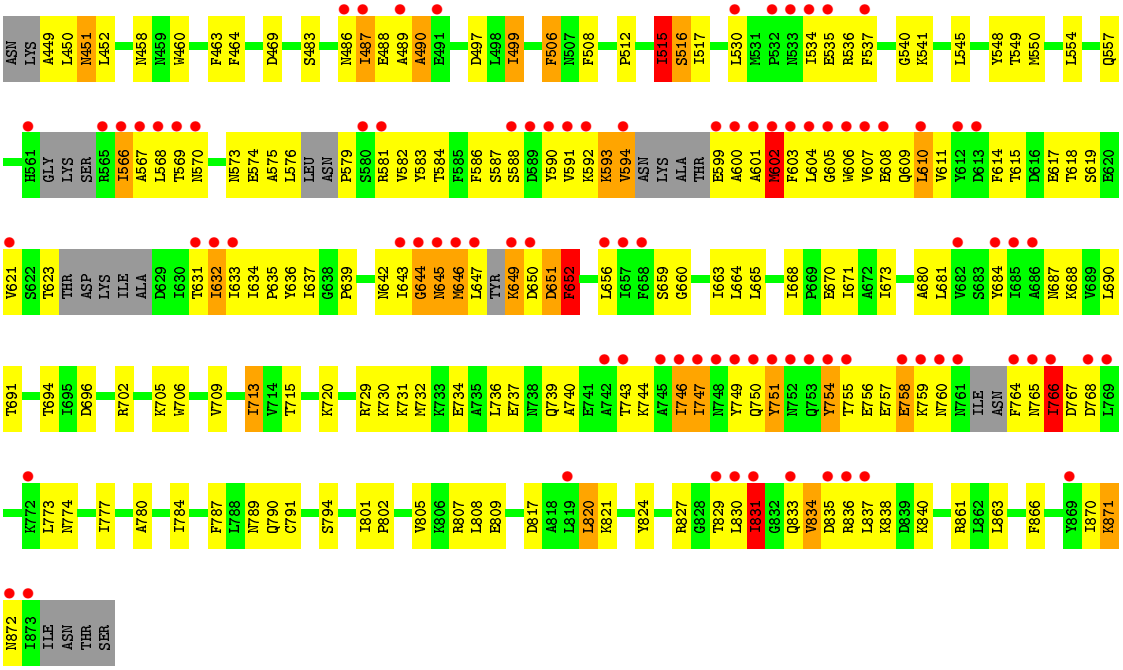
Chain B:





- Molecule 2: BOTULINUM NEUROTOXIN A HEAVY CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.36Å 156.91Å 211.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.59 49.11 – 2.59	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.11-2.59) 91.1 (49.11-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.253 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 79768 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14160	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/3618	0.64	0/4896
1	C	0.51	0/3605	0.63	0/4879
2	B	0.48	0/3492	0.61	0/4735
2	D	0.45	0/3364	0.66	3/4552 (0.1%)
All	All	0.48	0/14079	0.64	3/19062 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	652	PHE	CB-CG-CD1	-9.74	113.98	120.80
2	D	652	PHE	CB-CG-CD2	6.02	125.02	120.80
2	D	831	ILE	CB-CA-C	-5.11	101.38	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3534	0	3471	108	0
1	C	3522	0	3467	79	0
2	B	3429	0	3392	136	0
2	D	3308	0	3258	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	2	0	0	1	0
5	D	1	0	0	0	0
6	A	18	0	9	1	0
6	B	12	0	6	0	0
7	C	4	0	3	0	0
8	A	110	0	0	4	0
8	B	49	0	0	3	0
8	C	118	0	0	1	0
8	D	31	0	0	4	0
All	All	14160	0	13606	534	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (534) 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)
2:D:831:ILE:CG2	2:D:831:ILE:O	1.67	1.35
1:A:200:LEU:HG	2:B:861:ARG:NH1	1.46	1.30
2:D:649:LYS:O	2:D:649:LYS:CD	1.89	1.21
1:A:202:VAL:O	1:A:204:THR:N	1.74	1.19
2:D:659:SER:HB2	2:D:663:ILE:HD11	1.22	1.18
1:C:395:THR:HG22	1:C:397:LEU:H	1.13	1.11
2:D:450:LEU:HD22	2:D:451:ASN:H	1.13	1.10
1:A:395:THR:HG22	1:A:397:LEU:H	1.15	1.08
2:D:566:ILE:HG12	2:D:567:ALA:H	1.12	1.08
2:D:660:GLY:O	2:D:663:ILE:HD13	1.53	1.08
1:A:202:VAL:HG23	1:A:203:ASP:N	1.64	1.06
2:D:866:PHE:CZ	2:D:870:ILE:HD11	1.91	1.04
1:A:202:VAL:CG2	1:A:203:ASP:H	1.69	1.04
1:A:202:VAL:O	1:A:205:ASN:N	1.94	1.01
2:D:584:THR:HG22	2:D:586:PHE:H	1.21	1.01
2:D:649:LYS:O	2:D:649:LYS:HD3	1.61	0.99
2:D:602:MET:HG2	2:D:603:PHE:CE1	1.98	0.98
1:A:200:LEU:HG	2:B:861:ARG:HH11	1.07	0.97
2:D:831:ILE:HG23	2:D:831:ILE:O	1.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG23	1:A:203:ASP:H	0.82	0.96
1:A:201:GLU:OE2	1:A:364:LYS:NZ	2.02	0.93
2:B:530:LEU:HD12	2:B:530:LEU:H	1.34	0.93
2:D:709:VAL:O	2:D:713:ILE:HD13	1.71	0.91
2:D:743:THR:O	2:D:747:ILE:HD13	1.71	0.91
2:D:829:THR:O	2:D:830:LEU:HD23	1.69	0.91
2:D:487:ILE:HD13	2:D:487:ILE:H	1.36	0.90
1:A:200:LEU:CG	2:B:861:ARG:NH1	2.34	0.90
2:D:566:ILE:HG12	2:D:567:ALA:N	1.86	0.88
2:D:635:PRO:HA	2:D:652:PHE:HE2	1.37	0.88
1:A:74:ASP:OD1	1:A:76:THR:HG22	1.74	0.88
2:D:833:GLN:O	2:D:835:ASP:N	2.09	0.86
2:D:450:LEU:HD13	2:D:451:ASN:N	1.90	0.86
1:C:395:THR:HG22	1:C:397:LEU:N	1.90	0.86
2:D:487:ILE:HG12	2:D:488:GLU:H	1.39	0.85
2:D:637:ILE:HG12	2:D:732:MET:HE3	1.59	0.85
1:C:184:GLN:OE1	1:C:231:ARG:HD3	1.77	0.85
1:C:249:ALA:HB3	1:C:252:GLU:HG3	1.59	0.85
2:D:450:LEU:HD22	2:D:451:ASN:N	1.91	0.84
2:D:757:GLU:HG3	2:D:760:ASN:HB3	1.59	0.84
2:D:831:ILE:HG22	2:D:831:ILE:O	1.74	0.83
2:D:766:ILE:HG12	2:D:767:ASP:H	1.43	0.83
2:D:566:ILE:CG1	2:D:567:ALA:H	1.91	0.83
2:D:649:LYS:O	2:D:649:LYS:HD2	1.78	0.82
2:D:602:MET:HG2	2:D:603:PHE:CD1	2.14	0.82
1:A:395:THR:CG2	1:A:397:LEU:H	1.93	0.82
1:A:7:GLN:HG2	1:A:7:GLN:O	1.80	0.82
2:B:588:SER:O	2:B:591:VAL:HG22	1.81	0.81
2:D:601:ALA:O	2:D:602:MET:HB3	1.80	0.80
1:C:164:GLU:OE2	1:C:166:LYS:HE2	1.80	0.80
1:A:-2:PHE:HB2	1:A:387:TYR:HE2	1.47	0.80
1:A:14:VAL:HG13	1:A:20:ALA:HA	1.64	0.80
1:A:45:ILE:HB	1:A:154:ILE:HG22	1.62	0.80
1:C:210:ALA:HB2	2:D:774:ASN:OD1	1.82	0.80
2:D:593:LYS:O	2:D:599:GLU:HB2	1.82	0.79
1:A:200:LEU:HG	2:B:861:ARG:HH12	1.46	0.79
1:C:45:ILE:HB	1:C:154:ILE:HG12	1.65	0.79
2:B:572:VAL:HG13	2:B:574:GLU:H	1.47	0.78
2:D:599:GLU:HG2	2:D:600:ALA:N	1.98	0.78
1:A:200:LEU:CG	2:B:861:ARG:HH11	1.92	0.78
2:D:554:LEU:HD11	2:D:731:LYS:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:649:LYS:O	2:D:649:LYS:CG	2.29	0.77
2:B:565:ARG:HE	2:B:565:ARG:HA	1.49	0.77
2:D:515:ILE:O	2:D:516:SER:HB3	1.82	0.77
2:D:483:SER:HA	2:D:694:THR:HG22	1.66	0.77
2:D:633:ILE:O	2:D:635:PRO:HD3	1.85	0.77
1:A:201:GLU:HG2	1:A:361:LEU:HD11	1.67	0.76
1:A:428:LEU:HD23	2:B:542:LYS:HG3	1.68	0.76
2:D:588:SER:O	2:D:591:VAL:HG22	1.86	0.75
2:D:659:SER:CB	2:D:663:ILE:HD11	2.12	0.75
2:D:833:GLN:O	2:D:836:ARG:N	2.18	0.75
2:D:568:LEU:HD11	2:D:594:VAL:C	2.07	0.74
2:D:866:PHE:CE2	2:D:870:ILE:HD11	2.22	0.74
2:D:601:ALA:O	2:D:602:MET:CB	2.36	0.74
2:B:565:ARG:HG3	2:B:749:TYR:HB2	1.70	0.74
1:A:63:PRO:HG2	1:A:64:GLU:H	1.52	0.73
2:D:635:PRO:HA	2:D:652:PHE:CE2	2.22	0.73
2:D:488:GLU:HG3	2:D:489:ALA:H	1.53	0.73
1:A:395:THR:HG22	1:A:397:LEU:N	1.98	0.72
2:D:487:ILE:HG12	2:D:488:GLU:N	2.03	0.72
1:A:68:VAL:O	1:A:420:THR:HG21	1.89	0.72
2:D:599:GLU:HB3	2:D:610:LEU:HD11	1.70	0.72
1:A:66:LYS:O	1:A:68:VAL:N	2.22	0.72
2:D:599:GLU:HG2	2:D:600:ALA:H	1.52	0.72
2:D:833:GLN:O	2:D:834:VAL:C	2.27	0.72
2:D:673:ILE:HG22	2:D:807:ARG:HG3	1.70	0.72
2:D:690:LEU:O	2:D:694:THR:HG23	1.89	0.72
1:A:199:SER:O	1:A:200:LEU:CD1	2.37	0.71
2:D:450:LEU:CD2	2:D:451:ASN:H	1.97	0.71
2:D:584:THR:CG2	2:D:586:PHE:H	2.03	0.71
1:C:45:ILE:HD12	1:C:154:ILE:HD11	1.71	0.71
2:B:647:LEU:HD12	8:B:2031:HOH:O	1.90	0.70
2:D:829:THR:HG22	2:D:829:THR:O	1.90	0.70
2:D:573:ASN:O	2:D:576:LEU:HD12	1.90	0.69
2:D:664:LEU:HD11	2:D:791:CYS:SG	2.33	0.69
1:C:23:LYS:HA	1:C:30:MET:CE	2.22	0.69
2:D:632:ILE:HD13	2:D:632:ILE:H	1.58	0.68
1:A:201:GLU:CG	1:A:361:LEU:HD11	2.23	0.68
2:D:687:ASN:N	2:D:829:THR:HG21	2.08	0.68
2:B:785:ASN:HB3	2:B:861:ARG:NH2	2.09	0.68
2:B:575:ALA:HB1	2:B:581:ARG:O	1.93	0.68
2:D:570:ASN:HD22	2:D:581:ARG:HD3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:866:PHE:O	2:D:870:ILE:HG12	1.93	0.68
2:D:487:ILE:CD1	2:D:487:ILE:H	2.05	0.68
2:D:515:ILE:HD11	2:D:517:ILE:HG23	1.76	0.68
1:A:202:VAL:CG2	1:A:203:ASP:N	2.39	0.68
2:B:563:LYS:HE2	2:B:563:LYS:HA	1.76	0.68
1:A:184:GLN:OE1	1:A:231:ARG:HD3	1.93	0.68
2:B:563:LYS:O	2:B:565:ARG:N	2.27	0.67
1:C:334:ASP:HB3	1:C:337:LYS:HB2	1.75	0.67
1:A:65:ALA:O	1:A:66:LYS:HB2	1.92	0.67
1:C:395:THR:CG2	1:C:397:LEU:H	1.99	0.67
1:A:66:LYS:O	1:A:68:VAL:HG22	1.95	0.67
2:B:627:ILE:HG12	2:B:657:ILE:HA	1.75	0.67
1:A:199:SER:O	1:A:200:LEU:HD12	1.95	0.67
2:D:870:ILE:O	2:D:871:LYS:HB2	1.94	0.66
1:A:201:GLU:HG3	1:A:361:LEU:CD1	2.25	0.66
1:A:202:VAL:O	1:A:203:ASP:C	2.34	0.66
2:B:785:ASN:HB3	2:B:861:ARG:HH22	1.59	0.66
2:D:566:ILE:HB	2:D:749:TYR:CE2	2.30	0.66
2:B:569:THR:HG23	2:B:584:THR:CG2	2.25	0.66
2:D:599:GLU:CG	2:D:600:ALA:N	2.57	0.66
1:A:201:GLU:O	1:A:202:VAL:C	2.34	0.66
2:D:619:SER:O	2:D:621:VAL:HG23	1.97	0.65
1:A:200:LEU:O	1:A:203:ASP:OD2	2.15	0.65
2:D:601:ALA:O	2:D:602:MET:SD	2.55	0.64
2:B:702:ARG:HD2	2:B:812:ASP:OD1	1.96	0.64
2:B:729:ARG:HB3	2:B:788:LEU:HD12	1.79	0.64
2:D:632:ILE:HD13	2:D:790:GLN:OE1	1.97	0.64
1:C:201:GLU:HG3	1:C:361:LEU:CD1	2.27	0.64
2:D:602:MET:CG	2:D:603:PHE:CE1	2.77	0.64
1:A:98:ILE:O	1:A:104:GLY:HA3	1.96	0.64
2:D:550:MET:CE	2:D:731:LYS:HG2	2.28	0.64
1:A:270:ASP:OD1	1:A:365:THR:HG23	1.97	0.64
2:D:780:ALA:O	2:D:784:ILE:HG12	1.98	0.64
2:B:553:TYR:OH	2:B:647:LEU:HB3	1.99	0.63
2:D:450:LEU:O	2:D:451:ASN:HB2	1.98	0.63
2:D:740:ALA:O	2:D:744:LYS:HG3	1.97	0.63
2:D:530:LEU:H	2:D:530:LEU:HD12	1.63	0.63
1:A:201:GLU:CG	1:A:361:LEU:CD1	2.76	0.63
2:B:697:ASN:O	2:B:701:LYS:HB2	1.98	0.63
2:B:584:THR:HG22	2:B:739:GLN:OE1	1.99	0.63
1:A:325:GLU:HA	1:A:330:LYS:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:LEU:H	2:D:530:LEU:CD1	2.12	0.62
2:D:644:GLY:O	2:D:645:ASN:C	2.37	0.62
2:B:634:ILE:HD12	2:B:784:ILE:HA	1.82	0.62
2:D:634:ILE:HB	2:D:637:ILE:HD12	1.82	0.62
2:D:734:GLU:HA	2:D:737:GLU:HG2	1.81	0.62
2:D:650:ASP:O	2:D:651:ASP:C	2.37	0.62
2:D:766:ILE:HG12	2:D:767:ASP:N	2.14	0.62
2:B:530:LEU:N	2:B:530:LEU:HD12	2.11	0.61
2:D:642:ASN:OD1	2:D:646:MET:HA	2.00	0.61
2:D:663:ILE:CD1	2:D:663:ILE:H	2.14	0.61
1:A:80:THR:HG22	1:A:82:ASN:H	1.65	0.61
2:B:464:PHE:CE2	2:B:466:PRO:HG3	2.35	0.61
1:A:34:LYS:HZ2	6:A:1436:GOL:H11	1.66	0.61
2:B:569:THR:HG23	2:B:584:THR:HG23	1.82	0.60
2:B:635:PRO:HB2	2:B:649:LYS:HB3	1.82	0.60
2:B:805:VAL:O	2:B:809:GLU:HG3	2.01	0.60
2:D:691:THR:CG2	2:D:830:LEU:HD11	2.32	0.60
2:D:647:LEU:O	2:D:650:ASP:HB3	2.01	0.60
2:D:688:LYS:NZ	2:D:831:ILE:HG22	2.16	0.60
2:D:730:LYS:HG2	8:D:2024:HOH:O	2.02	0.59
1:A:202:VAL:C	1:A:204:THR:N	2.54	0.59
2:D:483:SER:CA	2:D:694:THR:HG22	2.32	0.59
2:B:646:MET:C	2:B:647:LEU:HD23	2.22	0.59
2:B:714:VAL:O	2:B:718:LEU:HB2	2.03	0.59
2:D:515:ILE:HD13	2:D:516:SER:H	1.67	0.59
2:B:671:ILE:HG23	2:B:671:ILE:O	2.03	0.59
2:D:691:THR:HG21	2:D:830:LEU:HD11	1.83	0.59
2:D:805:VAL:O	2:D:809:GLU:HG3	2.03	0.58
2:D:736:LEU:HB3	2:D:777:ILE:HD12	1.85	0.58
2:D:663:ILE:HD12	2:D:663:ILE:H	1.69	0.58
2:D:668:ILE:H	2:D:668:ILE:HD12	1.67	0.58
2:D:550:MET:CE	2:D:731:LYS:HE2	2.32	0.58
2:B:706:TRP:CE3	2:B:808:LEU:HD13	2.39	0.58
1:C:249:ALA:HB3	1:C:252:GLU:CG	2.33	0.58
2:B:560:GLU:C	2:B:562:GLY:H	2.07	0.58
1:C:431:VAL:HG21	2:D:548:TYR:HE2	1.69	0.58
1:C:257:GLU:HG3	2:D:534:ILE:HG23	1.84	0.57
2:B:553:TYR:CE2	2:B:642:ASN:HB2	2.40	0.57
1:A:421:GLY:H	1:A:424:GLU:HG3	1.69	0.57
1:C:201:GLU:HG2	1:C:364:LYS:HZ3	1.70	0.57
2:B:689:VAL:HG12	2:B:693:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD12	2:B:785:ASN:ND2	2.19	0.57
2:B:860:GLN:CD	2:B:860:GLN:H	2.08	0.57
2:D:671:ILE:O	2:D:671:ILE:HG23	2.04	0.57
1:A:199:SER:O	1:A:200:LEU:HD13	2.04	0.57
1:A:200:LEU:HD13	2:B:729:ARG:HD3	1.87	0.57
1:C:23:LYS:HA	1:C:30:MET:HE2	1.87	0.57
2:D:489:ALA:O	2:D:490:ALA:HB3	2.05	0.56
2:B:559:PHE:HE1	2:B:565:ARG:HH22	1.52	0.56
2:D:663:ILE:HD12	2:D:663:ILE:N	2.20	0.56
2:D:599:GLU:N	2:D:599:GLU:OE1	2.38	0.56
2:D:550:MET:HE3	2:D:731:LYS:HG2	1.87	0.56
1:C:272:LYS:O	2:D:715:THR:HG23	2.05	0.56
2:D:610:LEU:HD12	2:D:610:LEU:H	1.70	0.56
2:D:530:LEU:N	2:D:530:LEU:HD12	2.20	0.56
1:A:272:LYS:O	2:B:715:THR:HG23	2.06	0.56
1:C:348:ILE:HG12	2:D:499:ILE:HD12	1.88	0.56
2:D:593:LYS:O	2:D:594:VAL:HG13	2.04	0.55
2:D:594:VAL:HG13	2:D:610:LEU:HD21	1.88	0.55
2:D:834:VAL:O	2:D:838:LYS:HG3	2.06	0.55
1:C:201:GLU:HG3	1:C:361:LEU:HD11	1.87	0.55
2:D:541:LYS:HE2	2:D:541:LYS:HA	1.88	0.55
1:A:177:ARG:HD3	1:A:238:ASN:HA	1.87	0.55
2:D:644:GLY:O	2:D:646:MET:N	2.39	0.55
2:B:754:TYR:HB2	2:B:758:GLU:HG2	1.88	0.55
1:A:74:ASP:CG	1:A:76:THR:HG22	2.26	0.55
2:D:584:THR:HG22	2:D:586:PHE:N	2.05	0.55
2:D:554:LEU:CD1	2:D:731:LYS:HG3	2.37	0.54
2:D:637:ILE:HG23	2:D:732:MET:CE	2.37	0.54
2:D:637:ILE:HG23	2:D:732:MET:HE1	1.89	0.54
2:B:569:THR:HG22	2:B:591:VAL:HG12	1.88	0.54
2:B:565:ARG:NE	2:B:565:ARG:HA	2.20	0.54
2:D:540:GLY:O	2:D:541:LYS:C	2.45	0.54
1:C:348:ILE:HG12	2:D:499:ILE:CD1	2.36	0.54
1:C:39:HIS:CD2	1:C:40:ASN:N	2.75	0.54
1:C:125:THR:HA	8:C:2039:HOH:O	2.08	0.54
2:B:570:ASN:ND2	2:B:572:VAL:HG12	2.23	0.54
2:D:515:ILE:HD13	2:D:516:SER:N	2.23	0.54
2:B:553:TYR:CZ	2:B:642:ASN:HB2	2.43	0.54
1:A:201:GLU:HG3	1:A:361:LEU:HD13	1.89	0.53
2:D:590:TYR:OH	2:D:743:THR:HG21	2.07	0.53
1:C:115:ILE:HD11	2:D:512:PRO:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ILE:HG22	1:C:155:GLY:O	2.08	0.53
2:D:545:LEU:N	2:D:545:LEU:HD12	2.22	0.53
1:A:-3:GLU:HA	5:A:1435:CL:CL	2.45	0.53
2:D:696:ASP:OD2	2:D:840:LYS:HE2	2.08	0.53
1:C:67:GLN:HE22	2:D:537:PHE:H	1.56	0.53
2:B:729:ARG:HB3	2:B:788:LEU:CD1	2.38	0.53
2:B:755:THR:C	2:B:757:GLU:H	2.12	0.53
1:A:14:VAL:HG13	1:A:19:ILE:O	2.09	0.53
1:A:62:PRO:HG2	1:A:64:GLU:O	2.08	0.53
2:B:673:ILE:O	2:B:807:ARG:NH1	2.42	0.53
2:D:566:ILE:HB	2:D:749:TYR:CZ	2.44	0.53
2:B:530:LEU:O	2:B:531:MET:HB3	2.08	0.53
1:C:14:VAL:HA	1:C:19:ILE:HG22	1.91	0.53
2:B:497:ASP:O	2:B:500:GLN:HB3	2.08	0.53
2:B:778:ASN:O	2:B:782:ILE:HG13	2.09	0.53
2:B:687:ASN:ND2	2:B:690:LEU:HD22	2.23	0.53
1:C:255:GLY:HA3	2:D:537:PHE:CD2	2.43	0.53
2:D:450:LEU:C	2:D:450:LEU:HD13	2.29	0.53
2:B:679:PHE:CE2	2:B:701:LYS:HB3	2.45	0.53
1:A:381:LYS:HG2	8:A:2092:HOH:O	2.08	0.52
2:D:623:THR:O	2:D:623:THR:HG22	2.09	0.52
1:A:425:PHE:CZ	2:B:537:PHE:HB2	2.44	0.52
2:D:756:GLU:HG3	2:D:758:GLU:CD	2.30	0.52
2:D:634:ILE:HG21	2:D:784:ILE:CD1	2.40	0.52
2:B:471:PHE:CE2	2:B:720:LYS:HE3	2.45	0.52
2:D:643:ILE:HG22	2:D:663:ILE:HG22	1.91	0.52
2:D:583:TYR:CG	2:D:584:THR:N	2.77	0.52
2:D:687:ASN:H	2:D:829:THR:HG21	1.74	0.52
2:D:557:GLN:HA	2:D:582:VAL:HG13	1.90	0.52
1:C:422:LEU:O	1:C:423:PHE:CD1	2.63	0.52
1:C:249:ALA:O	1:C:427:LYS:NZ	2.42	0.52
1:C:230:HIS:CE1	1:C:264:ARG:HD3	2.44	0.52
2:B:567:ALA:O	2:B:568:LEU:HD22	2.11	0.51
2:D:668:ILE:N	2:D:668:ILE:HD12	2.25	0.51
2:D:535:GLU:CD	2:D:535:GLU:H	2.14	0.51
2:B:570:ASN:ND2	2:B:572:VAL:H	2.08	0.51
2:B:648:TYR:O	2:B:649:LYS:C	2.48	0.51
1:C:97:ARG:HA	1:C:386:ILE:HG23	1.91	0.51
1:C:23:LYS:HA	1:C:30:MET:HE1	1.90	0.51
2:D:569:THR:HG23	2:D:584:THR:OG1	2.10	0.51
2:B:702:ARG:HG3	2:B:811:PHE:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLY:N	1:A:424:GLU:HG3	2.25	0.51
2:B:593:LYS:NZ	2:B:609:GLN:HG3	2.27	0.51
1:C:115:ILE:HD11	2:D:512:PRO:CB	2.41	0.50
2:B:809:GLU:OE2	2:B:848:ASP:OD2	2.30	0.50
1:A:69:PRO:HG3	2:B:460:TRP:CD2	2.46	0.50
2:B:489:ALA:HA	2:D:872:ASN:O	2.12	0.50
2:D:684:TYR:CE1	2:D:694:THR:HG21	2.47	0.50
2:D:605:GLY:O	2:D:608:GLU:HB3	2.11	0.50
1:A:240:ASN:C	1:A:240:ASN:ND2	2.64	0.50
2:D:659:SER:HB2	2:D:663:ILE:CD1	2.16	0.50
2:D:450:LEU:CD1	2:D:451:ASN:N	2.69	0.50
2:D:610:LEU:HD13	2:D:747:ILE:HD11	1.94	0.50
2:B:600:ALA:HA	2:B:754:TYR:CZ	2.47	0.50
1:C:392:LEU:O	1:C:395:THR:HB	2.10	0.50
1:A:-2:PHE:HB2	1:A:387:TYR:CE2	2.37	0.50
1:C:181:GLY:HA2	1:C:231:ARG:O	2.11	0.50
2:D:739:GLN:NE2	2:D:739:GLN:HA	2.27	0.50
1:C:154:ILE:CG2	1:C:155:GLY:N	2.74	0.50
1:C:430:CYS:HB3	2:D:452:LEU:HB3	1.94	0.50
1:A:334:ASP:OD1	1:A:337:LYS:HG3	2.12	0.50
1:C:70:VAL:HG23	1:C:161:ILE:HD12	1.93	0.49
2:B:541:LYS:HG2	2:B:543:TYR:CE1	2.48	0.49
2:B:647:LEU:HB2	8:B:2031:HOH:O	2.12	0.49
1:A:102:ASP:O	1:A:106:MET:HG3	2.12	0.49
2:B:603:PHE:O	2:B:606:TRP:HB3	2.12	0.49
1:A:426:TYR:CE1	2:B:456:LYS:HG2	2.47	0.49
1:A:298:ASN:HD21	1:A:331:PHE:H	1.60	0.49
2:D:656:LEU:HD11	2:D:787:PHE:HZ	1.76	0.49
1:C:392:LEU:O	1:C:398:ALA:HB2	2.12	0.49
1:C:310:LEU:HG	1:C:314:LYS:HD2	1.94	0.49
2:D:602:MET:O	2:D:603:PHE:CB	2.61	0.49
2:D:592:LYS:C	2:D:594:VAL:H	2.15	0.49
1:A:200:LEU:HD12	2:B:785:ASN:CG	2.34	0.49
1:A:392:LEU:O	1:A:395:THR:HB	2.13	0.49
1:C:67:GLN:HG2	1:C:425:PHE:CE1	2.48	0.49
1:A:256:LEU:O	1:A:257:GLU:HB2	2.13	0.49
2:D:688:LYS:HZ1	2:D:831:ILE:HG22	1.77	0.48
2:B:706:TRP:CD2	2:B:808:LEU:HD13	2.48	0.48
2:D:636:TYR:C	2:D:639:PRO:HD2	2.32	0.48
2:D:757:GLU:CG	2:D:760:ASN:HB3	2.38	0.48
2:D:606:TRP:C	2:D:608:GLU:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:756:GLU:O	2:D:758:GLU:HG2	2.13	0.48
1:A:103:LEU:HD11	1:A:348:ILE:HG22	1.95	0.48
1:C:108:LEU:O	1:C:112:VAL:HG23	2.14	0.48
1:A:63:PRO:CG	1:A:64:GLU:H	2.24	0.48
2:B:751:TYR:CZ	2:B:758:GLU:HB3	2.49	0.48
1:C:67:GLN:OE1	2:D:536:ARG:HA	2.13	0.48
1:C:172:VAL:HG22	1:C:172:VAL:O	2.14	0.48
2:D:450:LEU:O	2:D:451:ASN:CB	2.61	0.48
1:A:14:VAL:CG1	1:A:20:ALA:HA	2.41	0.48
2:D:765:ASN:HD21	2:D:766:ILE:HD11	1.78	0.48
2:D:458:ASN:OD1	2:D:460:TRP:CD1	2.67	0.48
2:D:663:ILE:N	2:D:663:ILE:CD1	2.77	0.48
2:D:830:LEU:HD13	2:D:837:LEU:CD1	2.44	0.48
2:B:570:ASN:HD21	2:B:572:VAL:HG12	1.79	0.48
1:A:326:ASP:OD2	1:A:330:LYS:HB3	2.14	0.48
2:D:607:VAL:O	2:D:607:VAL:HG12	2.13	0.48
1:C:253:MET:HG3	2:D:463:PHE:O	2.14	0.48
1:A:344:MET:HE3	2:B:502:TYR:HD2	1.78	0.48
2:B:505:THR:HG22	1:C:204:THR:HG23	1.96	0.47
1:C:154:ILE:HG22	1:C:155:GLY:N	2.28	0.47
1:A:293:ILE:HD12	8:A:2044:HOH:O	2.13	0.47
2:B:765:ASN:OD1	2:B:767:ASP:HB2	2.14	0.47
2:B:754:TYR:HB2	2:B:758:GLU:CG	2.44	0.47
2:B:495:SER:HB2	2:D:497:ASP:OD2	2.14	0.47
2:D:576:LEU:C	2:D:579:PRO:HD2	2.35	0.47
2:B:627:ILE:CD1	2:B:633:ILE:HD11	2.45	0.47
2:B:633:ILE:HD13	2:B:656:LEU:HD23	1.97	0.47
1:C:285:TYR:CZ	1:C:289:LYS:HE3	2.50	0.47
1:C:395:THR:CG2	1:C:396:ASN:N	2.78	0.47
2:D:601:ALA:HB1	2:D:602:MET:HE1	1.96	0.47
2:D:834:VAL:HG12	2:D:838:LYS:HE3	1.97	0.47
1:C:0:SER:OG	1:C:1:MET:N	2.48	0.47
2:B:464:PHE:O	2:B:465:SER:HB3	2.15	0.47
2:B:681:LEU:HD22	2:B:681:LEU:N	2.29	0.47
2:D:817:ASP:O	2:D:821:LYS:HG3	2.14	0.47
2:B:685:ILE:O	2:B:686:ALA:HB3	2.14	0.47
2:D:550:MET:HE1	2:D:731:LYS:HG2	1.96	0.47
2:B:536:ARG:HG3	2:B:536:ARG:HH11	1.79	0.47
2:D:647:LEU:O	2:D:650:ASP:CB	2.63	0.47
2:B:537:PHE:CD2	2:B:537:PHE:N	2.81	0.47
1:A:262:GLU:HG2	1:A:366:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LYS:HE2	1:C:81:ASP:HB3	1.96	0.47
2:D:610:LEU:HD12	2:D:610:LEU:N	2.29	0.46
2:D:709:VAL:HG21	2:D:808:LEU:HD21	1.98	0.46
2:B:755:THR:O	2:B:757:GLU:N	2.48	0.46
1:C:351:GLU:O	1:C:355:VAL:HG23	2.15	0.46
1:A:252:GLU:O	2:B:462:LEU:HD13	2.15	0.46
1:C:98:ILE:O	1:C:104:GLY:HA3	2.15	0.46
2:D:833:GLN:C	8:D:2027:HOH:O	2.53	0.46
1:A:176:THR:HG21	1:A:231:ARG:NH1	2.30	0.46
2:B:653:VAL:O	2:B:657:ILE:HG13	2.15	0.46
2:D:499:ILE:N	2:D:499:ILE:HD13	2.30	0.46
1:A:126:GLU:HA	1:A:302:SER:O	2.15	0.46
2:D:602:MET:O	2:D:603:PHE:CD1	2.68	0.46
2:B:553:TYR:OH	2:B:647:LEU:HD13	2.15	0.46
1:A:240:ASN:C	1:A:240:ASN:HD22	2.19	0.46
1:C:284:LEU:C	1:C:284:LEU:HD13	2.36	0.46
1:A:220:THR:O	1:A:223:HIS:HB3	2.16	0.46
2:D:584:THR:HG23	2:D:739:GLN:OE1	2.16	0.46
1:C:67:GLN:HA	1:C:425:PHE:CE2	2.51	0.46
1:A:222:ALA:O	1:A:226:ILE:HG13	2.16	0.46
2:B:646:MET:O	2:B:647:LEU:HG	2.15	0.46
2:D:645:ASN:O	2:D:646:MET:O	2.33	0.46
1:A:49:ASP:HB2	1:A:154:ILE:HD12	1.98	0.46
1:C:243:PHE:CZ	1:C:273:PHE:HB3	2.51	0.46
2:D:670:GLU:O	2:D:720:LYS:NZ	2.47	0.46
2:D:550:MET:HE3	2:D:731:LYS:HE2	1.98	0.46
2:D:773:LEU:O	2:D:777:ILE:HG12	2.16	0.46
1:A:141:ASP:OD2	1:A:141:ASP:C	2.54	0.45
1:C:53:ASN:OD1	1:C:55:GLU:HB3	2.15	0.45
2:B:567:ALA:C	2:B:568:LEU:HD22	2.37	0.45
2:B:710:TYR:O	2:B:714:VAL:HG23	2.16	0.45
2:D:450:LEU:HD13	2:D:451:ASN:CA	2.47	0.45
1:A:23:LYS:HE3	2:B:522:SER:O	2.17	0.45
2:B:785:ASN:CB	2:B:861:ARG:HH22	2.28	0.45
2:D:706:TRP:CE3	2:D:808:LEU:HD13	2.51	0.45
1:A:387:TYR:CD2	1:C:0:SER:HB2	2.51	0.45
2:B:816:LYS:HA	2:B:845:LEU:HD12	1.97	0.45
2:B:567:ALA:HA	2:B:580:SER:O	2.17	0.45
2:D:861:ARG:NH2	8:D:2031:HOH:O	2.49	0.45
2:B:566:ILE:HG13	2:B:566:ILE:O	2.16	0.45
2:D:587:SER:HB3	2:D:617:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:680:ALA:C	2:D:681:LEU:HD12	2.37	0.45
1:A:201:GLU:O	1:A:202:VAL:O	2.35	0.45
2:D:593:LYS:O	2:D:610:LEU:HD21	2.16	0.45
2:B:560:GLU:O	2:B:562:GLY:N	2.47	0.45
2:B:831:ILE:HG23	2:B:832:GLY:N	2.31	0.45
2:D:606:TRP:C	2:D:608:GLU:N	2.70	0.45
2:D:584:THR:CG2	2:D:586:PHE:HB2	2.47	0.45
2:D:870:ILE:HG22	2:D:872:ASN:OD1	2.17	0.45
1:A:244:LYS:HG2	2:B:467:SER:OG	2.16	0.45
2:D:602:MET:HB3	2:D:750:GLN:NE2	2.32	0.44
2:D:637:ILE:HG12	2:D:732:MET:CE	2.40	0.44
2:D:576:LEU:O	2:D:579:PRO:HD2	2.16	0.44
2:B:464:PHE:HB3	8:B:2039:HOH:O	2.18	0.44
1:A:251:TYR:OH	2:B:667:PHE:HB3	2.16	0.44
2:D:765:ASN:O	2:D:766:ILE:C	2.54	0.44
1:C:201:GLU:OE2	1:C:201:GLU:HA	2.16	0.44
1:A:262:GLU:CG	1:A:366:TYR:CZ	3.00	0.44
2:D:614:PHE:O	2:D:618:THR:HG23	2.17	0.44
2:D:758:GLU:O	2:D:760:ASN:N	2.50	0.44
1:A:254:SER:N	2:B:459:ASN:OD1	2.43	0.44
1:C:259:SER:OG	1:C:262:GLU:HB2	2.17	0.44
2:D:506:PHE:HB3	2:D:508:PHE:CE1	2.52	0.44
2:D:575:ALA:HB1	2:D:581:ARG:CD	2.48	0.44
1:A:242:VAL:HA	1:A:259:SER:HA	2.00	0.44
2:D:764:PHE:HB2	2:D:768:ASP:CB	2.48	0.44
2:B:786:LYS:HE3	2:B:786:LYS:HB2	1.78	0.44
1:C:51:PHE:O	1:C:52:THR:C	2.56	0.44
2:D:751:TYR:O	2:D:754:TYR:HB2	2.17	0.44
2:D:702:ARG:O	2:D:705:LYS:HB3	2.18	0.44
2:D:631:THR:HB	2:D:790:GLN:HE22	1.80	0.44
1:C:67:GLN:HA	1:C:425:PHE:CZ	2.53	0.44
2:D:764:PHE:HB2	2:D:768:ASP:HB3	1.99	0.44
2:D:594:VAL:CG1	2:D:746:ILE:HG21	2.48	0.43
2:D:566:ILE:HD12	2:D:749:TYR:CD2	2.52	0.43
2:B:702:ARG:NH1	2:B:812:ASP:OD2	2.43	0.43
1:A:70:VAL:HA	1:A:418:ASN:HD21	1.83	0.43
1:C:374:PHE:CD1	1:C:415:LYS:HA	2.53	0.43
1:A:202:VAL:O	1:A:204:THR:CA	2.61	0.43
2:D:584:THR:HG21	2:D:586:PHE:HB2	2.01	0.43
2:D:746:ILE:O	2:D:749:TYR:HB3	2.18	0.43
2:D:601:ALA:C	2:D:602:MET:SD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:THR:CG2	2:B:591:VAL:HG12	2.48	0.43
2:D:535:GLU:OE2	2:D:535:GLU:N	2.41	0.43
1:C:284:LEU:HD22	1:C:284:LEU:O	2.18	0.43
2:D:450:LEU:CD2	2:D:451:ASN:N	2.70	0.43
2:D:747:ILE:H	2:D:747:ILE:CD1	2.32	0.43
2:D:729:ARG:NH2	2:D:789:ASN:OD1	2.51	0.43
1:A:241:ARG:HD3	8:A:2054:HOH:O	2.17	0.43
2:B:726:ASP:O	2:B:729:ARG:HG3	2.18	0.43
2:D:487:ILE:CG1	2:D:488:GLU:N	2.79	0.43
2:B:550:MET:HG3	2:B:641:LEU:HB3	2.00	0.43
2:B:702:ARG:HD3	2:B:845:LEU:HD22	2.01	0.43
1:C:322:LEU:HD12	1:C:341:LEU:HB2	2.00	0.43
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.19	0.43
2:D:739:GLN:O	2:D:743:THR:HG23	2.19	0.43
2:D:765:ASN:ND2	2:D:766:ILE:CD1	2.82	0.43
1:C:278:GLN:O	1:C:282:PHE:CD2	2.72	0.43
1:C:222:ALA:O	1:C:226:ILE:HG13	2.19	0.43
1:A:395:THR:CG2	1:A:396:ASN:N	2.82	0.42
2:D:747:ILE:N	2:D:747:ILE:CD1	2.82	0.42
2:D:673:ILE:CG2	2:D:807:ARG:HG3	2.44	0.42
2:D:530:LEU:CD1	2:D:530:LEU:N	2.79	0.42
2:B:854:SER:HA	2:B:863:LEU:HD21	2.00	0.42
2:B:530:LEU:O	2:B:531:MET:CB	2.67	0.42
2:D:645:ASN:O	2:D:646:MET:C	2.57	0.42
2:B:833:GLN:NE2	2:B:836:ARG:HH21	2.17	0.42
2:D:801:ILE:N	2:D:802:PRO:CD	2.83	0.42
2:D:824:TYR:O	2:D:827:ARG:HG2	2.19	0.42
2:B:866:PHE:O	2:B:869:TYR:HB3	2.19	0.42
2:D:601:ALA:O	2:D:602:MET:CG	2.67	0.42
2:D:834:VAL:CG1	2:D:838:LYS:HE3	2.49	0.42
1:C:39:HIS:CD2	1:C:40:ASN:H	2.37	0.42
2:B:733:LYS:O	2:B:737:GLU:HG3	2.19	0.42
2:D:602:MET:O	2:D:603:PHE:HB2	2.19	0.42
2:D:599:GLU:OE1	2:D:599:GLU:CA	2.68	0.42
2:B:536:ARG:NH1	2:B:536:ARG:HG3	2.34	0.42
2:B:702:ARG:HD3	2:B:845:LEU:CD2	2.50	0.42
1:A:117:PHE:HA	1:A:317:PHE:CE1	2.55	0.42
1:A:198:GLU:HA	1:A:198:GLU:OE2	2.19	0.42
2:B:628:ALA:O	2:B:629:ASP:HB2	2.19	0.42
2:D:820:LEU:HA	2:D:820:LEU:HD12	1.81	0.42
2:D:634:ILE:HG21	2:D:784:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:758:GLU:C	2:D:760:ASN:H	2.23	0.42
2:B:627:ILE:HD12	2:B:633:ILE:HD11	2.00	0.42
2:D:574:GLU:OE2	2:D:574:GLU:N	2.40	0.42
1:A:2:GLU:HG3	1:A:99:TYR:HE2	1.85	0.42
1:C:393:ARG:HA	1:C:398:ALA:HB2	2.02	0.41
2:D:765:ASN:HD21	2:D:766:ILE:CD1	2.33	0.41
1:C:379:VAL:HB	1:C:380:PRO:HD3	2.02	0.41
2:D:833:GLN:C	2:D:835:ASP:N	2.73	0.41
2:D:681:LEU:HD12	2:D:681:LEU:N	2.35	0.41
1:A:423:PHE:CD1	1:A:423:PHE:N	2.81	0.41
1:C:201:GLU:HG2	1:C:364:LYS:NZ	2.35	0.41
2:B:659:SER:OG	2:B:663:ILE:HD11	2.20	0.41
2:D:515:ILE:O	2:D:516:SER:CB	2.56	0.41
2:B:679:PHE:HE2	2:B:701:LYS:HB3	1.83	0.41
2:D:601:ALA:HB1	2:D:602:MET:CE	2.51	0.41
2:D:573:ASN:C	2:D:575:ALA:N	2.74	0.41
1:A:184:GLN:NE2	1:A:231:ARG:HB3	2.35	0.41
1:A:97:ARG:HA	1:A:386:ILE:HG23	2.02	0.41
2:D:450:LEU:HD13	2:D:451:ASN:CG	2.40	0.41
2:D:713:ILE:N	2:D:713:ILE:CD1	2.83	0.41
2:B:671:ILE:HD11	2:B:713:ILE:HG12	2.02	0.41
2:D:545:LEU:HD22	2:D:549:THR:CG2	2.51	0.41
1:C:170:HIS:CD2	1:C:171:GLU:HG2	2.56	0.41
1:C:235:ILE:HA	1:C:286:TYR:CE1	2.56	0.41
2:D:691:THR:HG22	2:D:830:LEU:HD11	2.03	0.41
2:D:790:GLN:O	2:D:794:SER:HB2	2.21	0.41
2:D:569:THR:HG23	2:D:584:THR:CB	2.51	0.41
2:D:691:THR:HB	2:D:830:LEU:HD21	2.03	0.41
2:B:553:TYR:CD2	2:B:642:ASN:HB2	2.56	0.41
2:B:633:ILE:CD1	2:B:656:LEU:HD23	2.51	0.41
1:A:226:ILE:HG22	1:A:230:HIS:CE1	2.56	0.41
2:B:834:VAL:HG23	2:B:835:ASP:N	2.34	0.41
2:D:566:ILE:O	2:D:567:ALA:HB2	2.21	0.41
2:B:591:VAL:HG23	2:B:592:LYS:N	2.36	0.41
2:D:684:TYR:HE1	2:D:694:THR:HG21	1.84	0.41
1:A:80:THR:HG22	1:A:81:ASP:N	2.36	0.41
1:C:69:PRO:HG3	2:D:460:TRP:CD2	2.56	0.41
1:C:242:VAL:HG12	1:C:243:PHE:N	2.36	0.41
1:C:10:TYR:HB2	1:C:85:ASP:HA	2.03	0.41
2:B:554:LEU:HD12	2:B:554:LEU:HA	1.91	0.41
2:B:859:ASN:OD1	2:B:862:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:756:GLU:O	2:D:758:GLU:N	2.51	0.41
2:B:563:LYS:O	2:B:564:SER:C	2.60	0.41
2:B:627:ILE:O	2:B:628:ALA:HB3	2.20	0.41
1:A:117:PHE:HE1	1:A:297:LEU:HD21	1.86	0.41
1:C:102:ASP:HB2	1:C:357:PHE:CE2	2.56	0.41
2:B:859:ASN:OD1	2:B:861:ARG:HG2	2.21	0.40
2:B:627:ILE:HD11	2:B:657:ILE:HG12	2.02	0.40
1:A:322:LEU:O	1:A:337:LYS:HE3	2.20	0.40
1:A:344:MET:HG3	1:A:348:ILE:HD12	2.03	0.40
2:D:575:ALA:HB1	2:D:581:ARG:HD2	2.04	0.40
1:A:293:ILE:CD1	8:A:2044:HOH:O	2.69	0.40
2:B:775:GLU:O	2:B:779:LYS:HG3	2.21	0.40
2:D:660:GLY:O	2:D:663:ILE:CD1	2.45	0.40
2:D:488:GLU:O	2:D:489:ALA:HB3	2.20	0.40
2:B:565:ARG:CG	2:B:749:TYR:HB2	2.46	0.40
1:A:103:LEU:HA	1:A:106:MET:HE2	2.02	0.40
1:C:223:HIS:ND1	1:C:351:GLU:OE1	2.54	0.40
2:B:599:GLU:OE1	2:B:599:GLU:N	2.35	0.40
1:A:145:ARG:HA	2:B:519:ASN:OD1	2.21	0.40
2:D:870:ILE:O	2:D:871:LYS:CB	2.67	0.40
2:D:634:ILE:HG13	2:D:784:ILE:HD13	2.04	0.40
2:D:634:ILE:HB	2:D:637:ILE:CD1	2.50	0.40
2:D:449:ALA:N	8:D:2003:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	405 (93%)	23 (5%)	7 (2%)	12	24
1	C	434/450 (96%)	408 (94%)	24 (6%)	2 (0%)	34	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	422/431 (98%)	379 (90%)	29 (7%)	14 (3%)	5 7
2	D	394/431 (91%)	341 (86%)	34 (9%)	19 (5%)	3 3
All	All	1685/1762 (96%)	1533 (91%)	110 (6%)	42 (2%)	7 12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ALA
1	A	66	LYS
1	A	67	GLN
1	A	202	VAL
1	A	203	ASP
2	B	464	PHE
2	B	564	SER
2	B	759	LYS
2	D	566	ILE
2	D	602	MET
2	D	645	ASN
2	D	646	MET
2	D	759	LYS
2	D	831	ILE
2	D	834	VAL
1	A	211	GLY
2	B	530	LEU
2	B	566	ILE
2	B	756	GLU
2	B	831	ILE
1	C	74	ASP
2	D	451	ASN
2	D	644	GLY
2	D	766	ILE
2	D	871	LYS
2	B	561	HIS
2	D	490	ALA
2	D	593	LYS
2	D	651	ASP
2	D	751	TYR
1	A	74	ASP
2	B	531	MET
2	B	628	ALA
2	B	833	GLN

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Mol	Chain	Res	Type
2	B	859	ASN
1	C	52	THR
2	B	761	ASN
2	D	516	SER
2	D	464	PHE
2	D	611	VAL
2	B	671	ILE
2	D	515	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/402 (97%)	380 (97%)	10 (3%)	54	80
1	C	389/402 (97%)	383 (98%)	6 (2%)	72	90
2	B	385/393 (98%)	370 (96%)	15 (4%)	39	68
2	D	372/393 (95%)	346 (93%)	26 (7%)	19	37
All	All	1536/1590 (97%)	1479 (96%)	57 (4%)	41	69

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLU
1	A	51	PHE
1	A	170	HIS
1	A	203	ASP
1	A	240	ASN
1	A	243	PHE
1	A	257	GLU
1	A	365	THR
1	A	395	THR
1	A	423	PHE
2	B	469	ASP
2	B	484	ASP
2	B	509	ASP

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Mol	Chain	Res	Type
2	B	530	LEU
2	B	541	LYS
2	B	548	TYR
2	B	561	HIS
2	B	563	LYS
2	B	565	ARG
2	B	647	LEU
2	B	650	ASP
2	B	659	SER
2	B	761	ASN
2	B	807	ARG
2	B	869	TYR
1	C	51	PHE
1	C	165	CYS
1	C	207	LEU
1	C	240	ASN
1	C	243	PHE
1	C	284	LEU
2	D	469	ASP
2	D	486	ASN
2	D	487	ILE
2	D	499	ILE
2	D	506	PHE
2	D	515	ILE
2	D	594	VAL
2	D	602	MET
2	D	604	LEU
2	D	609	GLN
2	D	610	LEU
2	D	615	THR
2	D	632	ILE
2	D	649	LYS
2	D	652	PHE
2	D	665	LEU
2	D	713	ILE
2	D	746	ILE
2	D	747	ILE
2	D	754	TYR
2	D	755	THR
2	D	758	GLU
2	D	766	ILE
2	D	820	LEU

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Mol	Chain	Res	Type
2	D	831	ILE
2	D	863	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	40	ASN
1	A	86	ASN
1	A	170	HIS
1	A	311	GLN
2	B	501	GLN
2	B	570	ASN
2	B	722	ASN
2	B	761	ASN
2	B	763	ASN
2	B	789	ASN
2	B	843	ASN
2	B	852	GLN
1	C	29	GLN
1	C	82	ASN
1	C	170	HIS
1	C	174	ASN
1	C	269	HIS
1	C	394	ASN
2	D	557	GLN
2	D	693	GLN
2	D	765	ASN
2	D	843	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	SO4	A	1433	-	4,4,4	0.30	0	6,6,6	0.09	0
6	GOL	A	1436	-	5,5,5	4.83	5 (100%)	5,5,5	5.72	3 (60%)
6	GOL	A	1437	-	5,5,5	4.73	5 (100%)	5,5,5	5.72	3 (60%)
6	GOL	A	1438	-	5,5,5	4.83	5 (100%)	5,5,5	5.66	3 (60%)
3	SO4	B	1872	-	4,4,4	0.27	0	6,6,6	0.09	0
6	GOL	B	1873	-	5,5,5	4.74	5 (100%)	5,5,5	5.68	3 (60%)
6	GOL	B	1874	-	5,5,5	4.80	5 (100%)	5,5,5	5.67	3 (60%)
7	ACT	C	1435	-	1,3,3	1.66	0	0,3,3	0.00	-
3	SO4	C	1436	-	4,4,4	0.28	0	6,6,6	0.08	0
3	SO4	C	1437	-	4,4,4	0.20	0	6,6,6	0.08	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	SO4	A	1433	-	-	0/0/0/0	0/0/0/0
6	GOL	A	1436	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1437	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1438	-	-	0/4/4/4	0/0/0/0
3	SO4	B	1872	-	-	0/0/0/0	0/0/0/0
6	GOL	B	1873	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1874	-	-	0/4/4/4	0/0/0/0
7	ACT	C	1435	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1436	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	1437	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1438	GOL	C3-C2	-8.21	1.20	1.52
6	B	1873	GOL	C3-C2	-8.20	1.21	1.52
6	B	1874	GOL	C3-C2	-8.16	1.21	1.52
6	A	1436	GOL	C3-C2	-8.13	1.21	1.52
6	A	1437	GOL	C3-C2	-8.09	1.21	1.52
6	B	1874	GOL	O1-C1	-4.60	1.22	1.42
6	A	1438	GOL	O1-C1	-4.54	1.22	1.42
6	A	1436	GOL	O1-C1	-4.49	1.23	1.42
6	A	1437	GOL	O1-C1	-4.31	1.23	1.42
6	B	1873	GOL	O1-C1	-4.24	1.24	1.42
6	A	1436	GOL	C1-C2	-3.24	1.39	1.52
6	A	1438	GOL	C1-C2	-3.21	1.40	1.52
6	B	1874	GOL	C1-C2	-3.13	1.40	1.52
6	A	1437	GOL	C1-C2	-3.10	1.40	1.52
6	A	1436	GOL	O2-C2	-2.88	1.34	1.43
6	A	1438	GOL	O2-C2	-2.84	1.35	1.43
6	B	1873	GOL	O2-C2	-2.82	1.35	1.43
6	A	1437	GOL	O2-C2	-2.80	1.35	1.43
6	B	1873	GOL	C1-C2	-2.79	1.41	1.52
6	B	1874	GOL	O2-C2	-2.72	1.35	1.43
6	A	1438	GOL	O3-C3	3.20	1.56	1.42
6	B	1874	GOL	O3-C3	3.24	1.56	1.42
6	A	1437	GOL	O3-C3	3.27	1.56	1.42
6	B	1873	GOL	O3-C3	3.35	1.56	1.42
6	A	1436	GOL	O3-C3	3.36	1.56	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1436	GOL	O1-C1-C2	3.19	125.66	110.18
6	A	1438	GOL	O1-C1-C2	3.21	125.77	110.18
6	B	1874	GOL	O1-C1-C2	3.24	125.89	110.18
6	A	1437	GOL	O1-C1-C2	3.35	126.45	110.18
6	B	1873	GOL	O1-C1-C2	3.45	126.93	110.18
6	A	1437	GOL	O2-C2-C3	6.44	138.19	108.65
6	B	1873	GOL	O2-C2-C3	6.46	138.28	108.65
6	A	1436	GOL	O2-C2-C3	6.57	138.76	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1438	GOL	O2-C2-C3	6.61	138.96	108.65
6	B	1874	GOL	O2-C2-C3	6.66	139.21	108.65
6	B	1874	GOL	O3-C3-C2	10.25	159.91	110.18
6	A	1438	GOL	O3-C3-C2	10.27	160.00	110.18
6	B	1873	GOL	O3-C3-C2	10.36	160.43	110.18
6	A	1436	GOL	O3-C3-C2	10.47	160.97	110.18
6	A	1437	GOL	O3-C3-C2	10.49	161.04	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1436	GOL	1	0

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, 95^{th} 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	437/450 (97%)	0.02	12 (2%) 58 51	12, 27, 54, 98	0
1	C	436/450 (96%)	0.02	9 (2%) 67 61	12, 30, 59, 75	0
2	B	424/431 (98%)	0.62	52 (12%) 5 3	20, 42, 78, 93	0
2	D	408/431 (94%)	1.18	90 (22%) 1 0	21, 48, 101, 117	0
All	All	1705/1762 (96%)	0.45	163 (9%) 10 6	12, 36, 78, 117	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	873	ILE	12.9
2	D	602	MET	9.8
2	D	764	PHE	8.8
2	D	755	THR	8.4
2	D	606	TRP	8.3
2	D	872	ASN	8.3
2	D	603	PHE	7.5
2	D	753	GLN	7.5
2	B	565	ARG	7.4
2	D	601	ALA	7.3
2	B	760	ASN	7.1
2	D	649	LYS	6.9
2	D	831	ILE	6.7
2	D	566	ILE	6.5
2	B	563	LYS	6.2
2	D	644	GLY	6.0
2	B	761	ASN	5.9
2	B	566	ILE	5.8
2	D	751	TYR	5.7
2	D	600	ALA	5.5
2	D	761	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	534	ILE	5.5
2	B	764	PHE	5.4
2	D	754	TYR	5.4
2	B	568	LEU	5.3
2	D	604	LEU	5.3
1	C	0	SER	5.3
2	D	830	LEU	5.3
1	A	-3	GLU	5.1
2	D	605	GLY	5.0
2	D	599	GLU	4.8
2	B	763	ASN	4.8
2	D	645	ASN	4.6
1	A	65	ALA	4.6
2	B	577	LEU	4.6
2	D	747	ILE	4.6
2	B	647	LEU	4.5
2	D	765	ASN	4.4
2	D	766	ILE	4.4
2	D	569	THR	4.3
2	B	537	PHE	4.3
2	D	658	PHE	4.3
1	A	64	GLU	4.3
2	D	533	ASN	4.2
2	D	565	ARG	4.1
2	D	750	GLN	4.1
2	B	762	ILE	4.0
2	D	607	VAL	4.0
1	C	64	GLU	4.0
2	D	833	GLN	3.9
2	D	837	LEU	3.9
2	D	568	LEU	3.8
2	D	746	ILE	3.8
2	B	755	THR	3.8
2	B	530	LEU	3.8
2	B	534	ILE	3.8
2	D	561	HIS	3.7
2	D	749	TYR	3.7
1	C	63	PRO	3.7
2	D	835	ASP	3.7
2	D	752	ASN	3.6
2	D	581	ARG	3.6
2	D	646	MET	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	831	ILE	3.6
2	B	564	SER	3.6
2	B	751	TYR	3.5
1	C	423	PHE	3.5
2	D	647	LEU	3.5
2	B	561	HIS	3.4
2	B	562	GLY	3.4
2	D	631	THR	3.4
2	B	533	ASN	3.4
2	D	608	GLU	3.3
2	D	836	ARG	3.3
2	B	752	ASN	3.3
2	D	829	THR	3.3
2	D	760	ASN	3.2
1	A	423	PHE	3.2
2	B	754	TYR	3.2
2	B	834	VAL	3.1
2	D	535	GLU	3.1
2	D	592	LYS	3.1
2	B	759	LYS	3.0
2	D	537	PHE	3.0
2	B	603	PHE	3.0
2	B	753	GLN	3.0
2	D	657	ILE	3.0
2	D	869	TYR	3.0
2	D	819	LEU	2.9
2	D	748	ASN	2.9
1	C	422	LEU	2.9
2	D	656	LEU	2.9
1	A	257	GLU	2.8
2	B	837	LEU	2.8
2	D	685	ILE	2.8
2	D	742	ALA	2.8
2	D	610	LEU	2.8
1	A	-2	PHE	2.7
2	D	591	VAL	2.7
2	B	756	GLU	2.7
2	B	870	ILE	2.7
2	D	768	ASP	2.7
1	A	200	LEU	2.7
2	B	599	GLU	2.6
2	D	530	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	759	LYS	2.6
2	B	597	ALA	2.6
2	D	487	ILE	2.6
2	B	532	PRO	2.6
2	D	633	ILE	2.6
2	D	594	VAL	2.6
2	D	612	TYR	2.5
1	A	425	PHE	2.5
2	B	765	ASN	2.5
2	D	588	SER	2.5
1	A	1	MET	2.5
1	A	202	VAL	2.5
2	D	567	ALA	2.5
2	D	632	ILE	2.5
2	B	803	TYR	2.5
2	D	758	GLU	2.5
2	B	629	ASP	2.4
2	D	613	ASP	2.4
1	C	171	GLU	2.4
2	B	823	ILE	2.4
2	B	490	ALA	2.3
2	B	766	ILE	2.3
2	B	648	TYR	2.3
2	B	758	GLU	2.3
2	B	681	LEU	2.3
2	D	745	ALA	2.2
2	B	690	LEU	2.2
2	D	621	VAL	2.2
2	B	682	VAL	2.2
2	B	869	TYR	2.2
2	B	806	LYS	2.2
2	D	772	LYS	2.2
2	D	743	THR	2.2
2	D	580	SER	2.2
2	D	589	ASP	2.2
2	D	650	ASP	2.2
2	D	489	ALA	2.2
1	A	63	PRO	2.2
2	B	824	TYR	2.1
2	D	491	GLU	2.1
2	D	643	ILE	2.1
2	B	596	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	860	GLN	2.1
2	B	658	PHE	2.1
2	D	486	ASN	2.1
2	D	769	LEU	2.1
2	B	604	LEU	2.1
2	D	532	PRO	2.1
1	A	0	SER	2.1
2	D	686	ALA	2.1
1	C	172	VAL	2.1
2	D	682	VAL	2.1
2	D	590	TYR	2.1
1	C	1	MET	2.0
2	D	570	ASN	2.0
2	B	600	ALA	2.0
1	C	203	ASP	2.0
2	D	684	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GOL	B	1874	6/6	0.92	0.16	3.59	55,59,59,60	0
7	ACT	C	1435	4/4	0.92	0.20	3.44	49,50,51,52	0
3	SO4	A	1433	5/5	0.92	0.20	2.68	68,69,70,72	0
6	GOL	A	1437	6/6	0.93	0.20	2.60	44,46,47,49	0
6	GOL	A	1436	6/6	0.88	0.17	1.70	54,55,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GOL	B	1873	6/6	0.80	0.20	1.64	51,53,55,56	0
3	SO4	C	1436	5/5	0.92	0.17	0.09	82,83,85,85	0
4	ZN	C	1438	1/1	1.00	0.18	-0.13	29,29,29,29	0
5	CL	A	1435	1/1	0.95	0.10	-0.75	44,44,44,44	0
3	SO4	C	1437	5/5	0.95	0.12	-0.92	69,69,70,70	0
3	SO4	B	1872	5/5	0.96	0.14	-1.74	47,48,50,51	0
4	ZN	A	1434	1/1	1.00	0.14	-1.75	23,23,23,23	0
6	GOL	A	1438	6/6	0.94	0.19	-	54,55,56,58	0
5	CL	A	1439	1/1	0.97	0.15	-	44,44,44,44	0
5	CL	D	1872	1/1	0.93	0.07	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.