



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:15 AM UTC

PDB ID : 1U22 / pdb_00001u22
Title : A. thaliana cobalamine independent methionine synthase
Authors : Ferrer, J.-L.; Ravanel, S.; Robert, M.; Dumas, R.
Deposited on : 2004-07-16
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

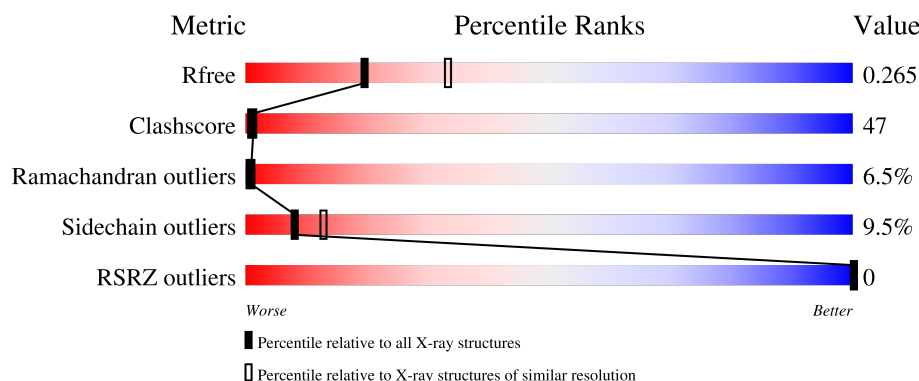
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	765	

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	769	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	THG	A	773	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6127 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	Se	0	0	0
			5783	3686	974	1099	6	18			

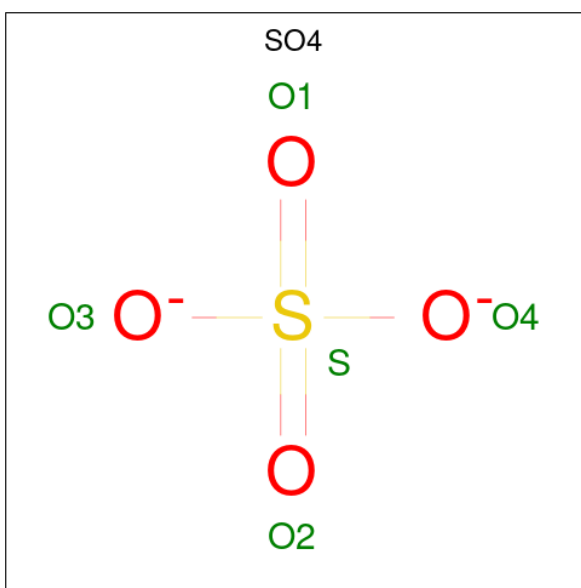
There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O50008
A	11	MSE	MET	modified residue	UNP O50008
A	49	MSE	MET	modified residue	UNP O50008
A	74	MSE	MET	modified residue	UNP O50008
A	97	MSE	MET	modified residue	UNP O50008
A	107	MSE	MET	modified residue	UNP O50008
A	109	MSE	MET	modified residue	UNP O50008
A	212	MSE	MET	modified residue	UNP O50008
A	351	MSE	LEU	modified residue	UNP O50008
A	496	MSE	MET	modified residue	UNP O50008
A	538	MSE	MET	modified residue	UNP O50008
A	545	MSE	MET	modified residue	UNP O50008
A	549	MSE	MET	modified residue	UNP O50008
A	554	MSE	MET	modified residue	UNP O50008
A	557	MSE	MET	modified residue	UNP O50008
A	648	MSE	MET	modified residue	UNP O50008
A	663	MSE	MET	modified residue	UNP O50008
A	718	MSE	MET	modified residue	UNP O50008
A	750	MSE	MET	modified residue	UNP O50008

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

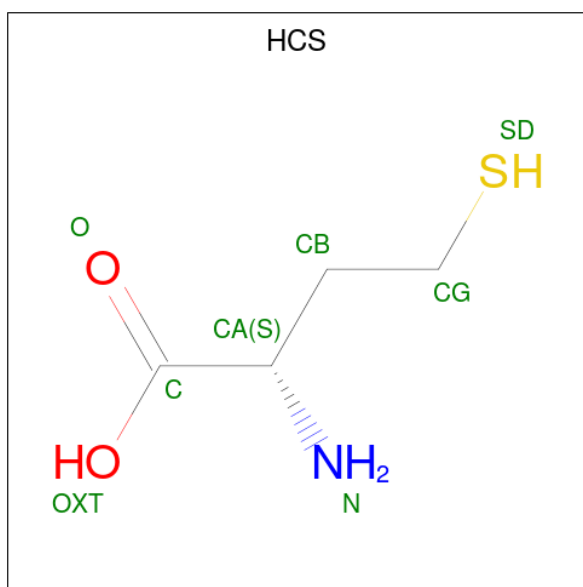
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



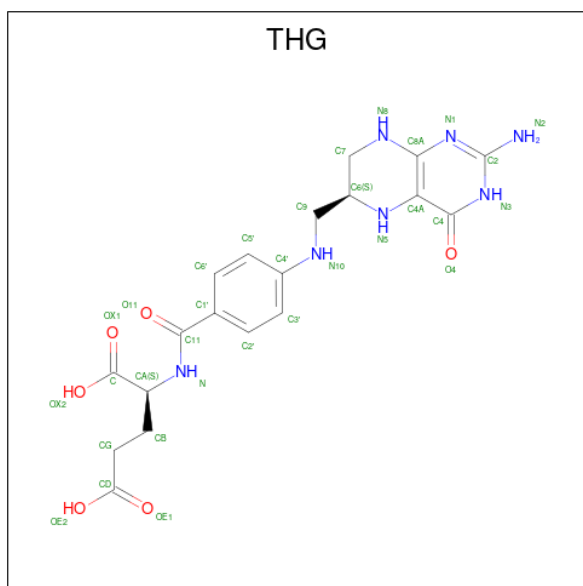
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (CCD ID: HCS) (formula: C₄H₉NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 5 is (6S)-5,6,7,8-TETRAHYDROFOLATE (CCD ID: THG) (formula: $C_{19}H_{23}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O		
			32	19	7	6	0	0

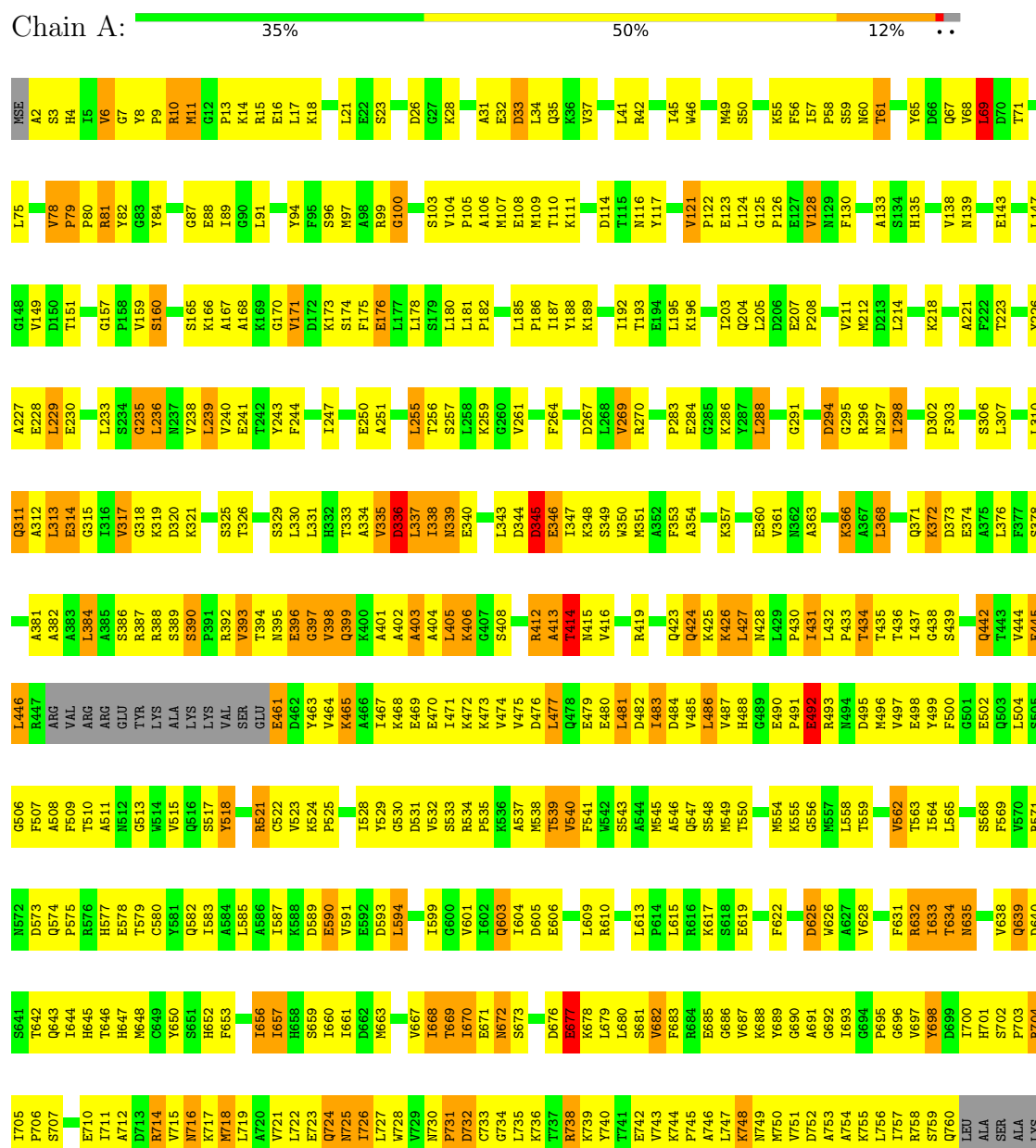
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	282	Total 282	O 282	0	0

3 Residue-property plots

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

- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	122.42Å 122.42Å 131.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.78 – 2.65 44.78 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.78-2.65) 99.8 (44.78-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.270 0.204 , 0.265	Depositor DCC
R_{free} test set	2910 reflections (8.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.117 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, THG, SO4, HCS

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	0/5884	1.05	35/7949 (0.4%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	GLY	N-CA-C	-9.98	99.99	113.37
1	A	594	LEU	N-CA-C	-9.31	101.92	113.18
1	A	269	VAL	N-CA-C	-8.31	104.42	111.56
1	A	716	ASN	N-CA-C	-7.37	104.81	113.88
1	A	718	MSE	N-CA-C	-7.22	104.45	113.55
1	A	732	ASP	N-CA-C	-7.17	105.14	114.04
1	A	677	GLU	N-CA-C	-7.08	104.68	113.38
1	A	227	ALA	N-CA-C	-7.00	103.26	111.03
1	A	78	VAL	CA-C-N	6.96	124.74	119.66
1	A	78	VAL	C-N-CA	6.96	124.74	119.66
1	A	313	LEU	N-CA-C	-6.77	103.83	111.07
1	A	556	GLY	N-CA-C	-6.35	104.63	111.93
1	A	384	LEU	N-CA-C	-6.34	104.29	111.14
1	A	714	ARG	N-CA-C	-6.25	104.36	112.23
1	A	61	THR	N-CA-C	-6.18	105.56	113.23
1	A	339	ASN	N-CA-C	-6.16	103.46	113.19
1	A	160	SER	N-CA-C	-6.13	104.60	111.28
1	A	682	VAL	N-CA-C	-6.12	105.33	112.98
1	A	437	ILE	N-CA-C	6.09	116.83	111.90
1	A	69	LEU	N-CA-C	-5.98	104.34	111.69
1	A	337	LEU	N-CA-C	-5.76	106.22	113.20
1	A	392	ARG	N-CA-C	-5.71	106.28	113.18
1	A	196	LYS	N-CA-C	-5.61	105.16	111.28
1	A	49	MSE	N-CA-C	5.43	117.01	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	LEU	N-CA-C	-5.42	106.43	113.16
1	A	79	PRO	CA-C-N	5.42	126.62	119.84
1	A	79	PRO	C-N-CA	5.42	126.62	119.84
1	A	704	ARG	N-CA-C	5.39	118.17	110.24
1	A	336	ASP	N-CA-C	5.35	117.24	108.52
1	A	701	HIS	N-CA-C	-5.28	106.52	113.17
1	A	404	ALA	N-CA-C	-5.27	106.83	113.20
1	A	295	GLY	N-CA-C	-5.26	106.56	115.34
1	A	593	ASP	N-CA-C	-5.12	107.58	113.88
1	A	335	VAL	N-CA-C	5.11	119.96	109.34
1	A	403	ALA	N-CA-C	-5.05	108.14	114.56

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	5783	0	5793	549	0
2	A	2	0	0	0	0
3	A	20	0	0	3	0
4	A	8	0	8	2	0
5	A	32	0	20	1	0
6	A	282	0	0	23	0
All	All	6127	0	5821	549	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 47.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HD12	1:A:431:ILE:H	1.23	1.00
1:A:538:MSE:HE2	1:A:590:GLU:HG3	1.41	0.98
1:A:346:GLU:O	1:A:349:SER:OG	1.80	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:TYR:HB3	1:A:744:LYS:HE2	1.43	0.97
1:A:212:MSE:HE1	1:A:615:LEU:HB3	1.46	0.97
1:A:230:GLU:HG3	1:A:259:LYS:HB3	1.45	0.96
1:A:739:LYS:HD3	1:A:740:TYR:N	1.83	0.93
1:A:366:LYS:HB3	1:A:371:GLN:HB2	1.47	0.93
1:A:480:GLU:HG3	1:A:481:LEU:HD23	1.51	0.92
1:A:350:TRP:HE1	1:A:386:SER:HB2	1.36	0.91
1:A:531:ASP:HA	1:A:582:GLN:HE22	1.35	0.90
1:A:185:LEU:HD23	1:A:228:GLU:HG2	1.55	0.89
1:A:628:VAL:HG13	1:A:663:MSE:HG2	1.51	0.89
1:A:667:VAL:HG22	1:A:692:GLY:HA3	1.54	0.89
1:A:676:ASP:HB2	1:A:679:LEU:HG	1.51	0.89
1:A:738:ARG:HE	1:A:738:ARG:HA	1.36	0.87
1:A:562:VAL:HB	1:A:606:GLU:OE2	1.76	0.85
1:A:110:THR:HG22	1:A:121:VAL:HG12	1.59	0.84
1:A:680:LEU:HB3	1:A:722:LEU:HD21	1.61	0.82
1:A:695:PRO:HD2	1:A:718:MSE:HE3	1.61	0.82
1:A:496:MSE:HE1	1:A:563:THR:HG21	1.61	0.81
1:A:739:LYS:HD3	1:A:740:TYR:H	1.45	0.81
1:A:604:ILE:O	1:A:646:THR:HA	1.82	0.80
1:A:384:LEU:HD22	1:A:388:ARG:NH2	1.96	0.79
1:A:398:VAL:O	1:A:398:VAL:HG12	1.81	0.78
1:A:667:VAL:HA	1:A:692:GLY:O	1.83	0.78
1:A:523:VAL:O	1:A:525:PRO:HD3	1.84	0.78
1:A:677:GLU:HG3	1:A:717:LYS:HD2	1.65	0.78
1:A:718:MSE:HA	1:A:721:VAL:HG22	1.67	0.77
1:A:444:VAL:HG23	1:A:445:GLU:H	1.49	0.77
1:A:661:ILE:HD13	1:A:689:TYR:HD1	1.49	0.77
1:A:446:LEU:N	1:A:446:LEU:HD22	1.99	0.76
1:A:605:ASP:OD1	4:A:772:HCS:HB2	1.85	0.76
1:A:446:LEU:HD22	1:A:446:LEU:H	1.51	0.75
1:A:661:ILE:HD13	1:A:689:TYR:CD1	2.22	0.75
1:A:7:GLY:HA2	1:A:61:THR:HG21	1.68	0.75
1:A:748:LYS:O	1:A:751:VAL:HG12	1.87	0.75
1:A:738:ARG:HA	1:A:738:ARG:NE	2.02	0.75
1:A:157:GLY:HA3	1:A:207:GLU:CD	2.13	0.74
1:A:211:VAL:HG23	1:A:212:MSE:HE3	1.70	0.73
1:A:698:TYR:O	1:A:732:ASP:HB2	1.89	0.73
1:A:310:LEU:HA	1:A:313:LEU:HD12	1.71	0.73
1:A:680:LEU:HD13	1:A:722:LEU:HD11	1.69	0.73
1:A:416:VAL:HG23	1:A:419:ARG:HH21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HB2	1:A:751:VAL:HG11	1.71	0.72
1:A:495:ASP:HB3	1:A:498:GLU:HB2	1.72	0.72
1:A:531:ASP:HA	1:A:582:GLN:NE2	2.04	0.71
1:A:69:LEU:HD21	1:A:97:MSE:HE3	1.71	0.71
1:A:426:LYS:HE3	1:A:426:LYS:HA	1.70	0.71
1:A:111:LYS:HD2	1:A:111:LYS:N	2.05	0.71
1:A:718:MSE:HE2	1:A:727:LEU:HD11	1.73	0.70
1:A:250:GLU:HB2	6:A:857:HOH:O	1.90	0.70
1:A:126:PRO:HG3	1:A:175:PHE:CE1	2.26	0.70
1:A:532:VAL:HG21	1:A:583:ILE:HG12	1.74	0.70
1:A:6:VAL:HG13	1:A:326:THR:OG1	1.92	0.69
1:A:571:ARG:HD2	1:A:573:ASP:OD1	1.92	0.69
1:A:124:LEU:O	1:A:167:ALA:HA	1.93	0.69
1:A:473:LYS:HZ1	1:A:491:PRO:HB3	1.58	0.69
1:A:716:ASN:ND2	1:A:757:ILE:HD12	2.08	0.69
1:A:583:ILE:O	1:A:587:ILE:HG12	1.93	0.68
1:A:233:LEU:HG	1:A:238:VAL:HG21	1.75	0.68
1:A:473:LYS:NZ	1:A:491:PRO:HB3	2.07	0.68
1:A:423:GLN:NE2	1:A:643:GLN:HA	2.09	0.68
1:A:442:GLN:HE22	1:A:736:LYS:HE3	1.59	0.68
1:A:521:ARG:HB3	5:A:773:THG:HC61	1.75	0.68
1:A:212:MSE:HE1	1:A:615:LEU:CB	2.21	0.68
1:A:477:LEU:HD23	1:A:483:ILE:HD13	1.76	0.68
1:A:533:SER:O	1:A:535:PRO:HD3	1.92	0.68
1:A:396:GLU:O	1:A:399:GLN:HB3	1.93	0.67
1:A:539:THR:HG22	1:A:543:SER:OG	1.95	0.67
1:A:353:PHE:O	1:A:357:LYS:HG3	1.95	0.67
1:A:485:VAL:CG1	1:A:555:LYS:HG3	2.25	0.67
1:A:109:MSE:HE1	1:A:518:TYR:CE1	2.29	0.67
1:A:464:VAL:HG13	1:A:465:LYS:HZ2	1.60	0.67
1:A:487:VAL:HG22	1:A:555:LYS:HB2	1.77	0.67
1:A:513:GLY:O	1:A:524:LYS:HG3	1.95	0.67
1:A:477:LEU:HB3	1:A:486:LEU:HD22	1.77	0.67
1:A:480:GLU:HG3	1:A:481:LEU:CD2	2.23	0.66
1:A:434:THR:HG22	1:A:750:MSE:HE3	1.78	0.66
1:A:208:PRO:O	1:A:211:VAL:HG22	1.96	0.66
1:A:235:GLY:O	1:A:236:LEU:HB2	1.96	0.66
1:A:719:LEU:HD23	1:A:727:LEU:HD23	1.76	0.66
1:A:591:VAL:HG21	1:A:634:THR:HG23	1.76	0.66
1:A:468:LYS:O	1:A:472:LYS:HG3	1.95	0.65
1:A:721:VAL:HG23	1:A:722:LEU:HG	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:N	1:A:106:ALA:HB2	2.11	0.65
1:A:546:ALA:CB	1:A:554:MSE:HE2	2.25	0.65
1:A:239:LEU:HD11	1:A:241:GLU:HG2	1.77	0.65
1:A:431:ILE:H	1:A:431:ILE:CD1	1.99	0.65
1:A:444:VAL:HG23	1:A:445:GLU:N	2.11	0.65
1:A:26:ASP:HB3	1:A:28:LYS:HE2	1.77	0.65
1:A:656:ILE:O	1:A:660:ILE:HD13	1.96	0.65
1:A:108:GLU:O	1:A:121:VAL:HG13	1.97	0.65
1:A:545:MSE:O	1:A:549:MSE:HE3	1.97	0.64
1:A:702:SER:OG	1:A:704:ARG:HG2	1.97	0.64
1:A:656:ILE:O	1:A:656:ILE:HG12	1.97	0.64
1:A:498:GLU:O	1:A:502:GLU:HG3	1.98	0.64
1:A:8:TYR:CD2	1:A:9:PRO:HD2	2.33	0.64
1:A:718:MSE:HB3	1:A:727:LEU:HD21	1.78	0.64
1:A:671:GLU:O	1:A:672:ASN:HB2	1.97	0.64
1:A:350:TRP:NE1	1:A:386:SER:HB2	2.12	0.64
1:A:431:ILE:HG22	1:A:432:LEU:HD13	1.78	0.64
1:A:122:PRO:HD2	1:A:165:SER:HA	1.80	0.63
1:A:714:ARG:HA	1:A:717:LYS:HE3	1.80	0.63
1:A:507:PHE:C	1:A:529:TYR:HE2	2.06	0.63
1:A:510:THR:O	1:A:524:LYS:NZ	2.25	0.63
1:A:336:ASP:CG	1:A:338:ILE:HG22	2.24	0.63
1:A:481:LEU:HD12	1:A:751:VAL:HB	1.79	0.63
1:A:487:VAL:HG12	1:A:488:HIS:N	2.15	0.62
1:A:685:GLU:C	1:A:687:VAL:H	2.07	0.62
1:A:343:LEU:HD11	1:A:510:THR:HG22	1.82	0.62
1:A:395:ASN:OD1	1:A:396:GLU:N	2.30	0.62
1:A:537:ALA:HA	1:A:590:GLU:OE2	2.00	0.62
1:A:603:GLN:HE21	1:A:647:HIS:HB2	1.64	0.62
1:A:605:ASP:HB3	1:A:647:HIS:HB3	1.81	0.62
1:A:469:GLU:HG3	1:A:473:LYS:HE3	1.80	0.62
1:A:318:GLY:C	1:A:320:ASP:H	2.07	0.62
1:A:311:GLN:O	1:A:314:GLU:HB2	1.99	0.62
1:A:515:VAL:O	1:A:522:CYS:HB3	2.00	0.62
1:A:751:VAL:O	1:A:755:LYS:HG3	2.00	0.62
1:A:481:LEU:HB2	1:A:751:VAL:CG1	2.30	0.61
1:A:648:MSE:HE1	1:A:660:ILE:HG13	1.82	0.61
1:A:705:ILE:HD11	1:A:742:GLU:HA	1.81	0.61
1:A:707:SER:HB2	1:A:710:GLU:HG3	1.81	0.61
1:A:326:THR:HG21	1:A:330:LEU:HD21	1.83	0.61
1:A:477:LEU:HD13	1:A:486:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:VAL:HG22	1:A:755:LYS:HE3	1.81	0.61
1:A:575:PRO:HB2	1:A:577:HIS:CE1	2.35	0.60
1:A:534:ARG:HG3	1:A:538:MSE:SE	2.50	0.60
1:A:718:MSE:CE	1:A:727:LEU:HD11	2.30	0.60
1:A:110:THR:HG22	1:A:121:VAL:CG1	2.31	0.60
1:A:397:GLY:C	1:A:399:GLN:H	2.08	0.60
1:A:669:THR:HG21	6:A:935:HOH:O	2.00	0.60
1:A:337:LEU:HD13	1:A:353:PHE:CE1	2.37	0.60
1:A:506:GLY:HA3	1:A:530:GLY:O	2.01	0.60
1:A:668:ILE:HG23	1:A:693:ILE:HD12	1.82	0.60
1:A:350:TRP:CZ2	1:A:387:ARG:HA	2.37	0.60
1:A:413:ALA:O	1:A:414:THR:C	2.44	0.60
1:A:188:TYR:O	1:A:192:ILE:HG13	2.02	0.60
1:A:344:ASP:O	1:A:348:LYS:HG3	2.01	0.60
1:A:748:LYS:HB2	1:A:748:LYS:NZ	2.17	0.60
1:A:749:ASN:HA	1:A:752:ASP:OD2	2.02	0.60
1:A:204:GLN:HG3	1:A:239:LEU:HD12	1.84	0.59
1:A:433:PRO:HA	1:A:484:ASP:OD2	2.01	0.59
1:A:471:ILE:HG13	1:A:475:VAL:HG23	1.84	0.59
1:A:211:VAL:HG23	1:A:212:MSE:CE	2.31	0.59
1:A:239:LEU:CD1	1:A:241:GLU:HG2	2.32	0.59
1:A:424:GLN:OE1	1:A:428:ASN:HA	2.03	0.59
1:A:445:GLU:OE1	1:A:445:GLU:HA	2.03	0.59
1:A:26:ASP:CB	1:A:28:LYS:HE2	2.33	0.59
1:A:435:THR:CG2	1:A:730:ASN:HB3	2.33	0.58
1:A:587:ILE:O	1:A:591:VAL:HG23	2.03	0.58
1:A:695:PRO:HD2	1:A:718:MSE:CE	2.32	0.58
1:A:696:GLY:HA2	1:A:731:PRO:O	2.02	0.58
1:A:78:VAL:HG11	1:A:84:TYR:CD2	2.38	0.58
1:A:343:LEU:HB2	1:A:348:LYS:HE2	1.84	0.58
1:A:471:ILE:O	1:A:475:VAL:HG23	2.04	0.58
1:A:477:LEU:HD23	1:A:483:ILE:CD1	2.32	0.58
1:A:740:TYR:O	1:A:744:LYS:HG3	2.03	0.58
1:A:756:LEU:HD12	1:A:760:GLN:HE22	1.69	0.58
1:A:4:HIS:HB2	1:A:56:PHE:HB2	1.86	0.58
1:A:431:ILE:HD12	1:A:431:ILE:N	2.06	0.58
1:A:14:LYS:HE2	1:A:339:ASN:ND2	2.19	0.58
1:A:477:LEU:HD22	1:A:486:LEU:HB3	1.86	0.57
1:A:485:VAL:HG12	1:A:555:LYS:HG3	1.86	0.57
1:A:577:HIS:HB3	1:A:626:TRP:CD2	2.40	0.57
1:A:135:HIS:O	1:A:139:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:HIS:HB3	1:A:626:TRP:CG	2.40	0.57
1:A:645:HIS:HA	1:A:667:VAL:O	2.04	0.57
1:A:716:ASN:HA	1:A:719:LEU:CD1	2.34	0.57
1:A:14:LYS:HE2	1:A:339:ASN:HD21	1.70	0.57
1:A:546:ALA:HB3	1:A:554:MSE:HE2	1.85	0.57
1:A:412:ARG:O	1:A:414:THR:N	2.38	0.57
1:A:435:THR:O	1:A:750:MSE:HE1	2.04	0.57
1:A:517:SER:O	1:A:518:TYR:HB3	2.03	0.57
1:A:138:VAL:HG12	6:A:969:HOH:O	2.04	0.56
1:A:176:GLU:HG3	6:A:1020:HOH:O	2.04	0.56
1:A:435:THR:O	1:A:731:PRO:HD3	2.04	0.56
1:A:181:LEU:O	1:A:185:LEU:HB2	2.05	0.56
1:A:464:VAL:HG13	1:A:465:LYS:NZ	2.20	0.56
1:A:578:GLU:O	1:A:582:GLN:HG3	2.05	0.56
1:A:67:GLN:O	1:A:71:THR:HG22	2.04	0.56
1:A:432:LEU:HA	1:A:727:LEU:O	2.05	0.56
1:A:479:GLU:HG3	1:A:480:GLU:N	2.21	0.56
1:A:712:ALA:HB2	1:A:753:ALA:CB	2.34	0.56
1:A:599:ILE:N	1:A:599:ILE:HD12	2.20	0.56
1:A:255:LEU:HD22	1:A:264:PHE:CD1	2.41	0.56
1:A:228:GLU:O	1:A:228:GLU:HG3	2.05	0.56
1:A:495:ASP:OD2	1:A:498:GLU:HG3	2.05	0.56
1:A:464:VAL:CG1	1:A:465:LYS:HZ2	2.19	0.56
1:A:685:GLU:O	1:A:687:VAL:N	2.39	0.56
1:A:714:ARG:NH1	1:A:714:ARG:HB3	2.21	0.56
1:A:506:GLY:O	1:A:528:ILE:HA	2.05	0.56
1:A:439:SER:HB2	1:A:736:LYS:HB2	1.88	0.55
1:A:714:ARG:HG2	1:A:717:LYS:HE3	1.89	0.55
1:A:59:SER:HB3	1:A:151:THR:CB	2.36	0.55
1:A:307:LEU:O	1:A:311:GLN:HB2	2.06	0.55
1:A:638:VAL:HG22	1:A:642:THR:HB	1.86	0.55
1:A:203:ILE:HG12	1:A:204:GLN:H	1.71	0.55
1:A:402:ALA:HA	1:A:405:LEU:HD23	1.89	0.55
1:A:498:GLU:O	1:A:499:TYR:C	2.49	0.55
1:A:685:GLU:C	1:A:687:VAL:N	2.61	0.55
1:A:719:LEU:HD11	1:A:757:ILE:HG21	1.89	0.55
1:A:2:ALA:HB1	1:A:55:LYS:HG2	1.88	0.55
1:A:677:GLU:O	1:A:721:VAL:HG21	2.06	0.55
1:A:181:LEU:N	1:A:182:PRO:CD	2.70	0.55
1:A:399:GLN:C	1:A:399:GLN:CD	2.74	0.55
1:A:714:ARG:HG2	1:A:717:LYS:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD13	1:A:747:LEU:O	2.07	0.55
1:A:559:THR:HA	1:A:605:ASP:OD2	2.07	0.55
1:A:303:PHE:H	1:A:303:PHE:HD1	1.53	0.54
1:A:399:GLN:C	1:A:401:ALA:H	2.13	0.54
1:A:603:GLN:HB2	1:A:645:HIS:HB2	1.89	0.54
1:A:716:ASN:HA	1:A:719:LEU:HG	1.89	0.54
1:A:754:ALA:O	1:A:758:ARG:HG3	2.07	0.54
1:A:752:ASP:HA	1:A:755:LYS:HD2	1.88	0.54
1:A:111:LYS:HD2	1:A:111:LYS:H	1.72	0.54
1:A:59:SER:HB3	1:A:151:THR:OG1	2.08	0.54
1:A:125:GLY:O	1:A:128:VAL:HG12	2.08	0.54
1:A:481:LEU:CB	1:A:751:VAL:HG11	2.36	0.54
1:A:203:ILE:HG12	1:A:204:GLN:N	2.22	0.54
1:A:317:VAL:HG11	1:A:321:LYS:HB2	1.89	0.54
1:A:338:ILE:HG23	1:A:338:ILE:O	2.07	0.54
1:A:469:GLU:O	1:A:473:LYS:HG3	2.07	0.54
1:A:123:GLU:HB3	1:A:168:ALA:HB2	1.89	0.54
1:A:363:ALA:HA	6:A:824:HOH:O	2.07	0.54
1:A:430:PRO:HG2	1:A:758:ARG:NH2	2.23	0.54
1:A:546:ALA:HB1	1:A:554:MSE:HE2	1.90	0.54
1:A:432:LEU:HD21	1:A:719:LEU:HD21	1.89	0.54
1:A:212:MSE:HE1	1:A:615:LEU:HD13	1.89	0.53
1:A:78:VAL:HG11	1:A:84:TYR:CB	2.37	0.53
1:A:643:GLN:O	1:A:644:ILE:HD13	2.08	0.53
1:A:381:ALA:HA	1:A:384:LEU:HD12	1.89	0.53
1:A:446:LEU:H	1:A:446:LEU:CD2	2.21	0.53
1:A:585:LEU:HD12	1:A:633:ILE:HG21	1.89	0.53
1:A:653:PHE:CE1	1:A:670:ILE:HD12	2.43	0.53
1:A:68:VAL:HA	1:A:71:THR:CG2	2.39	0.53
1:A:471:ILE:HD13	1:A:549:MSE:SE	2.59	0.53
1:A:635:ASN:O	1:A:638:VAL:HG12	2.09	0.53
1:A:344:ASP:O	1:A:348:LYS:HE3	2.08	0.53
1:A:157:GLY:HA3	1:A:207:GLU:OE1	2.09	0.53
1:A:46:TRP:HB3	1:A:149:VAL:HG11	1.91	0.53
1:A:11:MSE:HE1	6:A:902:HOH:O	2.09	0.53
1:A:23:SER:HA	1:A:26:ASP:OD2	2.09	0.53
1:A:617:LYS:HE2	6:A:883:HOH:O	2.08	0.53
1:A:58:PRO:HB3	6:A:789:HOH:O	2.08	0.52
1:A:700:ILE:HD13	1:A:734:GLY:O	2.09	0.52
1:A:78:VAL:HG11	1:A:84:TYR:CG	2.44	0.52
1:A:538:MSE:H	1:A:590:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:GLY:CA	1:A:731:PRO:O	2.57	0.52
1:A:401:ALA:C	1:A:403:ALA:H	2.16	0.52
1:A:431:ILE:HG22	1:A:432:LEU:CD1	2.40	0.52
1:A:739:LYS:HB2	1:A:742:GLU:OE2	2.09	0.52
1:A:363:ALA:HB2	1:A:376:LEU:HD13	1.92	0.52
1:A:715:VAL:HG12	1:A:715:VAL:O	2.09	0.52
1:A:678:LYS:HG3	6:A:840:HOH:O	2.10	0.52
1:A:689:TYR:CZ	1:A:691:ALA:HB3	2.45	0.52
1:A:493:ARG:NH1	1:A:500:PHE:HZ	2.07	0.52
1:A:712:ALA:HB2	1:A:753:ALA:HB1	1.92	0.52
1:A:726:ILE:HD12	1:A:726:ILE:C	2.35	0.52
1:A:310:LEU:HB3	1:A:368:LEU:HD11	1.91	0.52
1:A:336:ASP:OD1	1:A:338:ILE:HG22	2.08	0.52
1:A:442:GLN:HG2	1:A:445:GLU:HG3	1.90	0.52
1:A:298:ILE:HG23	1:A:298:ILE:O	2.09	0.52
1:A:485:VAL:HG11	1:A:555:LYS:HG3	1.91	0.52
1:A:35:GLN:HA	1:A:35:GLN:HE21	1.75	0.51
1:A:475:VAL:O	1:A:479:GLU:HG2	2.10	0.51
1:A:50:SER:HA	1:A:57:ILE:HD11	1.92	0.51
1:A:604:ILE:HD13	1:A:634:THR:HG21	1.92	0.51
1:A:681:SER:O	1:A:685:GLU:HB2	2.10	0.51
1:A:712:ALA:HB2	1:A:753:ALA:HA	1.92	0.51
1:A:648:MSE:CE	1:A:668:ILE:HD11	2.41	0.51
1:A:41:LEU:HD12	6:A:1043:HOH:O	2.10	0.51
1:A:753:ALA:O	1:A:757:ILE:HG12	2.10	0.51
1:A:680:LEU:HB3	1:A:722:LEU:CD2	2.36	0.51
1:A:14:LYS:CE	1:A:339:ASN:ND2	2.73	0.51
1:A:230:GLU:CG	1:A:259:LYS:HB3	2.28	0.51
1:A:306:SER:O	1:A:310:LEU:HG	2.10	0.51
1:A:434:THR:HB	1:A:483:ILE:HA	1.92	0.51
1:A:481:LEU:HB2	1:A:751:VAL:CB	2.40	0.51
1:A:594:LEU:HA	1:A:599:ILE:HD13	1.92	0.51
1:A:212:MSE:CE	1:A:615:LEU:HB3	2.32	0.51
1:A:496:MSE:HE2	1:A:497:VAL:HG23	1.91	0.51
1:A:715:VAL:O	1:A:719:LEU:HG	2.12	0.51
1:A:716:ASN:OD1	1:A:719:LEU:HD12	2.11	0.51
1:A:751:VAL:HG13	1:A:752:ASP:N	2.26	0.51
1:A:343:LEU:CB	1:A:348:LYS:HE2	2.40	0.50
1:A:718:MSE:HA	1:A:721:VAL:CG2	2.39	0.50
1:A:712:ALA:HA	1:A:715:VAL:HB	1.93	0.50
1:A:610:ARG:HB3	1:A:650:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:O	1:A:147:LEU:HD13	2.12	0.50
1:A:533:SER:C	1:A:535:PRO:HD3	2.37	0.50
1:A:212:MSE:HA	1:A:212:MSE:HE2	1.93	0.50
1:A:562:VAL:HG11	1:A:609:LEU:HA	1.93	0.50
1:A:622:PHE:O	1:A:625:ASP:HB3	2.12	0.50
1:A:89:ILE:HG13	1:A:133:ALA:HB1	1.92	0.50
1:A:126:PRO:HG3	1:A:175:PHE:CD1	2.47	0.50
1:A:11:MSE:CE	1:A:17:LEU:HD23	2.41	0.49
1:A:170:GLY:O	1:A:171:VAL:C	2.55	0.49
1:A:354:ALA:O	1:A:357:LYS:N	2.45	0.49
1:A:668:ILE:HG23	1:A:693:ILE:CD1	2.41	0.49
1:A:399:GLN:C	1:A:401:ALA:N	2.70	0.49
1:A:668:ILE:HG22	1:A:689:TYR:OH	2.13	0.49
1:A:693:ILE:HG22	1:A:726:ILE:HD13	1.94	0.49
1:A:477:LEU:HD22	1:A:486:LEU:HA	1.94	0.49
1:A:534:ARG:NH1	1:A:590:GLU:OE2	2.44	0.49
1:A:711:ILE:HG22	1:A:715:VAL:HG21	1.93	0.49
1:A:739:LYS:O	1:A:743:VAL:HG22	2.12	0.49
1:A:431:ILE:O	1:A:758:ARG:NE	2.46	0.49
1:A:688:LYS:O	1:A:688:LYS:HG2	2.12	0.49
1:A:337:LEU:HD12	1:A:340:GLU:CG	2.43	0.49
1:A:395:ASN:O	1:A:398:VAL:HB	2.12	0.49
1:A:474:VAL:C	1:A:476:ASP:N	2.70	0.49
1:A:645:HIS:CE1	1:A:667:VAL:HB	2.47	0.49
1:A:700:ILE:O	1:A:738:ARG:HD2	2.11	0.49
1:A:8:TYR:CE2	1:A:45:ILE:HD12	2.48	0.49
1:A:532:VAL:HG21	1:A:583:ILE:CG1	2.43	0.49
1:A:240:VAL:HG23	1:A:261:VAL:HG13	1.95	0.49
1:A:398:VAL:O	1:A:398:VAL:CG1	2.53	0.49
1:A:496:MSE:CE	1:A:497:VAL:HG23	2.43	0.49
1:A:705:ILE:CD1	1:A:742:GLU:HA	2.43	0.49
1:A:382:ALA:HA	6:A:1045:HOH:O	2.13	0.48
1:A:711:ILE:O	1:A:715:VAL:HG23	2.13	0.48
1:A:114:ASP:OD2	1:A:270:ARG:NH1	2.46	0.48
1:A:330:LEU:O	1:A:333:THR:HG22	2.13	0.48
1:A:751:VAL:CG1	1:A:752:ASP:N	2.77	0.48
1:A:173:LYS:HG3	1:A:174:SER:N	2.28	0.48
1:A:725:ASN:O	1:A:726:ILE:HG23	2.13	0.48
1:A:204:GLN:HG3	1:A:239:LEU:CD1	2.44	0.48
1:A:617:LYS:C	1:A:619:GLU:H	2.20	0.48
1:A:104:VAL:HG13	1:A:105:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:GLU:O	1:A:724:GLN:C	2.57	0.48
1:A:683:PHE:HD1	1:A:689:TYR:HB2	1.79	0.47
1:A:718:MSE:CA	1:A:721:VAL:HG22	2.42	0.47
1:A:340:GLU:OE1	1:A:511:ALA:N	2.42	0.47
1:A:653:PHE:HA	1:A:656:ILE:CG2	2.43	0.47
1:A:723:GLU:O	1:A:725:ASN:N	2.47	0.47
1:A:205:LEU:N	1:A:205:LEU:HD22	2.29	0.47
1:A:406:LYS:NZ	1:A:406:LYS:HB3	2.30	0.47
1:A:539:THR:O	1:A:541:PHE:N	2.48	0.47
1:A:515:VAL:HG21	1:A:569:PHE:HZ	1.80	0.47
1:A:318:GLY:C	1:A:320:ASP:N	2.73	0.47
1:A:633:ILE:HG22	1:A:633:ILE:O	2.13	0.47
1:A:676:ASP:HB3	6:A:840:HOH:O	2.14	0.47
1:A:13:PRO:HD2	1:A:16:GLU:OE2	2.15	0.47
1:A:685:GLU:O	1:A:687:VAL:HG23	2.15	0.47
1:A:75:LEU:HD23	1:A:187:ILE:HG21	1.96	0.46
1:A:84:TYR:OH	1:A:87:GLY:O	2.29	0.46
1:A:165:SER:O	1:A:166:LYS:HD3	2.14	0.46
1:A:372:LYS:O	1:A:374:GLU:N	2.47	0.46
1:A:491:PRO:HG2	1:A:492:GLU:H	1.79	0.46
1:A:702:SER:O	1:A:703:PRO:C	2.57	0.46
1:A:606:GLU:OE1	1:A:606:GLU:HA	2.15	0.46
1:A:679:LEU:O	1:A:682:VAL:HG13	2.15	0.46
1:A:432:LEU:N	1:A:433:PRO:CD	2.78	0.46
1:A:719:LEU:HD11	1:A:757:ILE:CG2	2.44	0.46
1:A:748:LYS:HB2	1:A:748:LYS:HZ2	1.80	0.46
1:A:714:ARG:HB3	1:A:714:ARG:CZ	2.45	0.46
1:A:218:LYS:O	1:A:221:ALA:HB3	2.15	0.46
1:A:481:LEU:O	1:A:751:VAL:HG21	2.16	0.46
1:A:166:LYS:HE2	6:A:812:HOH:O	2.15	0.46
1:A:69:LEU:HD13	1:A:94:TYR:CE1	2.51	0.46
1:A:212:MSE:CE	1:A:615:LEU:HD13	2.45	0.46
1:A:270:ARG:NH1	1:A:296:ARG:NH2	2.64	0.46
1:A:464:VAL:CG1	1:A:465:LYS:NZ	2.78	0.46
1:A:481:LEU:O	1:A:483:ILE:N	2.48	0.46
1:A:508:ALA:N	1:A:529:TYR:HE2	2.14	0.46
1:A:575:PRO:CB	1:A:577:HIS:CE1	2.99	0.46
1:A:33:ASP:O	1:A:37:VAL:HG23	2.16	0.46
1:A:294:ASP:OD2	1:A:297:ASN:HB2	2.15	0.46
1:A:632:ARG:O	1:A:634:THR:N	2.49	0.46
1:A:319:LYS:O	1:A:320:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:HB2	3:A:769:SO4:O2	2.16	0.46
1:A:461:GLU:N	1:A:464:VAL:HG12	2.31	0.45
1:A:17:LEU:HG	1:A:21:LEU:HG	1.98	0.45
1:A:388:ARG:HB2	6:A:832:HOH:O	2.16	0.45
1:A:590:GLU:O	1:A:594:LEU:HG	2.16	0.45
1:A:661:ILE:HG21	6:A:1003:HOH:O	2.16	0.45
1:A:605:ASP:HA	1:A:647:HIS:H	1.81	0.45
1:A:419:ARG:O	1:A:423:GLN:HG3	2.17	0.45
1:A:42:ARG:HG2	1:A:46:TRP:CH2	2.52	0.45
1:A:114:ASP:OD1	1:A:296:ARG:NH2	2.49	0.45
1:A:547:GLN:HE22	1:A:550:THR:HG23	1.82	0.45
1:A:96:SER:O	1:A:100:GLY:N	2.45	0.45
1:A:414:THR:HG21	1:A:640:ASP:OD1	2.17	0.45
1:A:705:ILE:HD12	1:A:745:PRO:HG2	1.97	0.45
1:A:79:PRO:CG	1:A:107:MSE:HE3	2.47	0.45
1:A:81:ARG:HG2	3:A:768:SO4:O3	2.16	0.45
1:A:255:LEU:C	1:A:257:SER:H	2.25	0.45
1:A:267:ASP:OD1	1:A:267:ASP:C	2.58	0.45
1:A:283:PRO:HB2	1:A:286:LYS:CG	2.47	0.45
1:A:434:THR:O	1:A:435:THR:HB	2.17	0.45
1:A:351:MSE:HE1	1:A:510:THR:CG2	2.47	0.45
1:A:681:SER:C	1:A:683:PHE:H	2.25	0.45
1:A:716:ASN:HA	1:A:719:LEU:CG	2.47	0.45
1:A:175:PHE:HZ	1:A:180:LEU:HD21	1.82	0.44
1:A:603:GLN:NE2	6:A:935:HOH:O	2.49	0.44
1:A:712:ALA:HB2	1:A:753:ALA:CA	2.47	0.44
1:A:99:ARG:C	1:A:106:ALA:HB2	2.42	0.44
1:A:238:VAL:HB	1:A:261:VAL:HA	1.99	0.44
1:A:444:VAL:CG2	1:A:445:GLU:H	2.24	0.44
1:A:589:ASP:C	1:A:591:VAL:N	2.75	0.44
1:A:653:PHE:O	1:A:657:ILE:N	2.50	0.44
1:A:15:ARG:O	1:A:18:LYS:HB3	2.17	0.44
1:A:211:VAL:HG12	1:A:247:ILE:CD1	2.46	0.44
1:A:334:ALA:HB3	1:A:353:PHE:CD2	2.53	0.44
1:A:470:GLU:HG3	1:A:491:PRO:HG3	1.99	0.44
1:A:639:GLN:HB2	1:A:642:THR:OG1	2.17	0.44
1:A:109:MSE:HE1	1:A:518:TYR:CD1	2.53	0.44
1:A:650:TYR:HB2	1:A:653:PHE:CZ	2.52	0.44
1:A:130:PHE:HB3	1:A:187:ILE:CD1	2.47	0.44
1:A:650:TYR:HB3	3:A:769:SO4:O4	2.18	0.44
1:A:69:LEU:CD2	1:A:97:MSE:HE3	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:O	1:A:244:PHE:HB2	2.18	0.44
1:A:384:LEU:HB3	1:A:388:ARG:CZ	2.47	0.44
1:A:648:MSE:HE3	1:A:670:ILE:HG22	1.99	0.44
1:A:463:TYR:CE1	1:A:541:PHE:CE2	3.06	0.44
1:A:631:PHE:O	1:A:634:THR:HB	2.17	0.44
1:A:32:GLU:HG2	6:A:998:HOH:O	2.18	0.44
1:A:298:ILE:HG13	1:A:353:PHE:CE1	2.53	0.44
1:A:389:SER:O	1:A:390:SER:C	2.61	0.44
1:A:397:GLY:C	1:A:399:GLN:N	2.76	0.44
1:A:59:SER:O	1:A:60:ASN:CB	2.66	0.43
1:A:79:PRO:HB2	1:A:82:TYR:CD2	2.53	0.43
1:A:185:LEU:N	1:A:186:PRO:CD	2.81	0.43
1:A:559:THR:HG22	1:A:564:ILE:HG13	2.00	0.43
1:A:632:ARG:C	1:A:634:THR:N	2.76	0.43
1:A:716:ASN:HA	1:A:719:LEU:HD12	2.00	0.43
1:A:735:LEU:HD11	1:A:747:LEU:HD11	2.00	0.43
1:A:10:ARG:NH2	1:A:117:TYR:OH	2.51	0.43
1:A:185:LEU:HG	1:A:229:LEU:CD1	2.49	0.43
1:A:426:LYS:HB3	1:A:427:LEU:HD23	2.00	0.43
1:A:589:ASP:O	1:A:591:VAL:N	2.51	0.43
1:A:288:LEU:C	1:A:288:LEU:HD23	2.43	0.43
1:A:414:THR:O	1:A:415:ASN:C	2.62	0.43
1:A:481:LEU:CD1	1:A:751:VAL:HB	2.46	0.43
1:A:487:VAL:CG1	1:A:488:HIS:N	2.78	0.43
1:A:659:SER:O	1:A:663:MSE:HG3	2.18	0.43
1:A:226:TYR:HA	1:A:229:LEU:HB2	2.00	0.43
1:A:558:LEU:CD1	1:A:591:VAL:HG22	2.48	0.43
1:A:96:SER:O	1:A:97:MSE:C	2.62	0.43
1:A:445:GLU:OE1	1:A:445:GLU:CA	2.65	0.43
1:A:603:GLN:HA	1:A:645:HIS:O	2.18	0.43
1:A:719:LEU:HD22	1:A:724:GLN:HG3	2.00	0.43
1:A:476:ASP:O	1:A:477:LEU:C	2.62	0.43
1:A:534:ARG:NH1	1:A:589:ASP:HB3	2.33	0.43
1:A:716:ASN:HD22	1:A:757:ILE:HD12	1.84	0.43
1:A:439:SER:CB	1:A:736:LYS:HB2	2.48	0.43
1:A:467:ILE:O	1:A:468:LYS:C	2.62	0.43
1:A:498:GLU:OE1	1:A:509:PHE:CE2	2.72	0.43
1:A:545:MSE:HG2	1:A:549:MSE:CE	2.48	0.43
1:A:465:LYS:O	1:A:468:LYS:HB3	2.19	0.43
1:A:687:VAL:O	1:A:688:LYS:HB3	2.19	0.43
1:A:4:HIS:O	1:A:325:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:HA	1:A:79:PRO:HD3	1.86	0.43
1:A:111:LYS:N	1:A:111:LYS:CD	2.78	0.43
1:A:251:ALA:HB2	6:A:873:HOH:O	2.18	0.43
1:A:259:LYS:C	1:A:261:VAL:H	2.27	0.43
1:A:343:LEU:CB	1:A:348:LYS:CE	2.96	0.43
1:A:360:GLU:O	1:A:361:VAL:C	2.61	0.43
1:A:416:VAL:HG23	1:A:419:ARG:NH2	2.27	0.43
1:A:435:THR:HG23	1:A:730:ASN:HB3	2.01	0.43
1:A:508:ALA:HB2	1:A:529:TYR:CE2	2.54	0.43
1:A:610:ARG:O	1:A:613:LEU:HB2	2.18	0.43
1:A:291:GLY:HA2	1:A:325:SER:O	2.18	0.43
1:A:605:ASP:CB	1:A:647:HIS:HB3	2.47	0.43
1:A:653:PHE:HA	1:A:656:ILE:HG22	2.01	0.43
1:A:446:LEU:N	1:A:446:LEU:CD2	2.71	0.42
1:A:547:GLN:HA	1:A:547:GLN:NE2	2.34	0.42
1:A:631:PHE:CZ	1:A:646:THR:HB	2.53	0.42
1:A:167:ALA:HB1	1:A:171:VAL:HG11	1.99	0.42
1:A:481:LEU:HB2	1:A:751:VAL:HB	2.00	0.42
1:A:68:VAL:HA	1:A:71:THR:HG22	2.01	0.42
1:A:223:THR:HG23	6:A:906:HOH:O	2.18	0.42
1:A:577:HIS:CG	1:A:578:GLU:N	2.88	0.42
1:A:587:ILE:C	1:A:589:ASP:N	2.76	0.42
1:A:347:ILE:HD13	1:A:347:ILE:HA	1.93	0.42
1:A:601:VAL:CG1	1:A:645:HIS:CD2	3.02	0.42
1:A:679:LEU:O	1:A:682:VAL:HG22	2.19	0.42
1:A:756:LEU:CD1	1:A:760:GLN:HE22	2.31	0.42
1:A:79:PRO:HA	1:A:80:PRO:HD3	1.84	0.42
1:A:243:TYR:HA	1:A:267:ASP:HB2	2.02	0.42
1:A:378:SER:HA	6:A:968:HOH:O	2.18	0.42
1:A:714:ARG:C	1:A:716:ASN:H	2.27	0.42
1:A:424:GLN:O	1:A:425:LYS:C	2.63	0.42
1:A:571:ARG:HD2	1:A:573:ASP:CG	2.43	0.42
1:A:671:GLU:HG2	1:A:672:ASN:H	1.84	0.42
1:A:738:ARG:HB3	1:A:743:VAL:HG13	2.00	0.42
1:A:755:LYS:O	1:A:758:ARG:HB2	2.20	0.42
1:A:435:THR:HG22	1:A:730:ASN:HB3	2.00	0.42
1:A:714:ARG:HA	1:A:717:LYS:CE	2.48	0.42
1:A:6:VAL:HG22	1:A:329:SER:HA	2.02	0.42
1:A:347:ILE:O	1:A:350:TRP:HB2	2.20	0.42
1:A:574:GLN:NE2	1:A:579:THR:OG1	2.47	0.42
1:A:13:PRO:HG2	6:A:940:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:C	1:A:315:GLY:H	2.28	0.41
1:A:430:PRO:HG2	1:A:758:ARG:HH22	1.84	0.41
1:A:539:THR:N	1:A:590:GLU:OE1	2.49	0.41
1:A:35:GLN:HA	1:A:35:GLN:NE2	2.35	0.41
1:A:255:LEU:HD22	1:A:264:PHE:CE1	2.55	0.41
1:A:302:ASP:O	1:A:303:PHE:C	2.62	0.41
1:A:186:PRO:O	1:A:189:LYS:HB2	2.20	0.41
1:A:353:PHE:N	1:A:353:PHE:CD1	2.88	0.41
1:A:395:ASN:CG	1:A:396:GLU:H	2.27	0.41
1:A:426:LYS:HA	1:A:426:LYS:CE	2.46	0.41
1:A:461:GLU:N	1:A:464:VAL:CG1	2.83	0.41
1:A:698:TYR:CE1	1:A:706:PRO:HD3	2.55	0.41
1:A:78:VAL:CG1	1:A:84:TYR:CD2	3.02	0.41
1:A:208:PRO:HB3	1:A:243:TYR:CE1	2.54	0.41
1:A:545:MSE:HG3	6:A:875:HOH:O	2.20	0.41
1:A:628:VAL:HG21	1:A:659:SER:HB3	2.03	0.41
1:A:68:VAL:O	1:A:71:THR:HG23	2.20	0.41
1:A:88:GLU:OE1	1:A:88:GLU:HA	2.20	0.41
1:A:314:GLU:O	1:A:317:VAL:O	2.39	0.41
1:A:433:PRO:HG2	1:A:728:TRP:CD2	2.55	0.41
1:A:204:GLN:CG	1:A:239:LEU:HD12	2.50	0.41
1:A:345:ASP:O	1:A:346:GLU:C	2.64	0.41
1:A:589:ASP:C	1:A:591:VAL:H	2.28	0.41
1:A:594:LEU:CA	1:A:599:ILE:HD13	2.50	0.41
1:A:724:GLN:HA	1:A:727:LEU:HB2	2.01	0.41
1:A:288:LEU:C	1:A:288:LEU:CD2	2.94	0.41
1:A:438:GLY:HA3	4:A:772:HCS:H2	1.85	0.41
1:A:714:ARG:HG2	1:A:717:LYS:NZ	2.36	0.41
1:A:31:ALA:O	1:A:32:GLU:C	2.64	0.41
1:A:160:SER:OG	1:A:207:GLU:HA	2.21	0.41
1:A:348:LYS:C	1:A:350:TRP:N	2.77	0.41
1:A:493:ARG:NH1	1:A:500:PHE:CZ	2.87	0.41
1:A:528:ILE:HG13	1:A:568:SER:OG	2.20	0.41
1:A:565:LEU:HD22	1:A:580:CYS:HB2	2.03	0.41
1:A:638:VAL:CG2	1:A:642:THR:HB	2.49	0.41
1:A:657:ILE:HD11	1:A:683:PHE:CE1	2.56	0.41
1:A:690:GLY:O	1:A:691:ALA:HB2	2.21	0.41
1:A:733:CYS:SG	1:A:734:GLY:N	2.94	0.41
1:A:756:LEU:O	1:A:759:SER:HB2	2.20	0.41
1:A:479:GLU:HG3	1:A:480:GLU:H	1.84	0.41
1:A:752:ASP:O	1:A:755:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ALA:O	1:A:405:LEU:CD2	2.68	0.40
1:A:603:GLN:CD	6:A:935:HOH:O	2.64	0.40
1:A:493:ARG:NH2	1:A:539:THR:HG23	2.37	0.40
1:A:617:LYS:C	1:A:619:GLU:N	2.80	0.40
1:A:396:GLU:OE1	1:A:396:GLU:CA	2.69	0.40
1:A:539:THR:HB	1:A:540:VAL:H	1.46	0.40
1:A:647:HIS:HA	1:A:669:THR:O	2.22	0.40
1:A:393:VAL:HG12	1:A:394:THR:N	2.37	0.40
1:A:412:ARG:O	1:A:413:ALA:C	2.64	0.40
1:A:697:VAL:HG11	1:A:715:VAL:HG22	2.02	0.40
1:A:743:VAL:HA	1:A:746:ALA:HB3	2.03	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.89	0.40
1:A:504:LEU:HD21	1:A:534:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	742/765 (97%)	581 (78%)	113 (15%)	48 (6%)	1 1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	LYS
1	A	413	ALA
1	A	414	THR
1	A	481	LEU
1	A	540	VAL
1	A	548	SER
1	A	672	ASN
1	A	725	ASN

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Mol	Chain	Res	Type
1	A	731	PRO
1	A	91	LEU
1	A	171	VAL
1	A	236	LEU
1	A	256	THR
1	A	335	VAL
1	A	345	ASP
1	A	373	ASP
1	A	398	VAL
1	A	408	SER
1	A	412	ARG
1	A	482	ASP
1	A	539	THR
1	A	656	ILE
1	A	698	TYR
1	A	726	ILE
1	A	235	GLY
1	A	294	ASP
1	A	346	GLU
1	A	492	GLU
1	A	518	TYR
1	A	590	GLU
1	A	639	GLN
1	A	724	GLN
1	A	81	ARG
1	A	100	GLY
1	A	633	ILE
1	A	686	GLY
1	A	65	TYR
1	A	103	SER
1	A	317	VAL
1	A	483	ILE
1	A	625	ASP
1	A	673	SER
1	A	284	GLU
1	A	490	GLU
1	A	390	SER
1	A	670	ILE
1	A	338	ILE
1	A	393	VAL

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	622/619 (100%)	563 (90%)	59 (10%)	8 13

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	VAL
1	A	10	ARG
1	A	11	MSE
1	A	33	ASP
1	A	34	LEU
1	A	69	LEU
1	A	116	ASN
1	A	121	VAL
1	A	128	VAL
1	A	159	VAL
1	A	176	GLU
1	A	178	LEU
1	A	193	THR
1	A	195	LEU
1	A	214	LEU
1	A	229	LEU
1	A	239	LEU
1	A	255	LEU
1	A	269	VAL
1	A	288	LEU
1	A	298	ILE
1	A	311	GLN
1	A	314	GLU
1	A	331	LEU
1	A	336	ASP
1	A	345	ASP
1	A	366	LYS
1	A	368	LEU
1	A	396	GLU

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Mol	Chain	Res	Type
1	A	399	GLN
1	A	406	LYS
1	A	414	THR
1	A	424	GLN
1	A	426	LYS
1	A	427	LEU
1	A	431	ILE
1	A	434	THR
1	A	436	THR
1	A	442	GLN
1	A	445	GLU
1	A	446	LEU
1	A	461	GLU
1	A	465	LYS
1	A	477	LEU
1	A	486	LEU
1	A	492	GLU
1	A	521	ARG
1	A	562	VAL
1	A	603	GLN
1	A	632	ARG
1	A	634	THR
1	A	635	ASN
1	A	657	ILE
1	A	668	ILE
1	A	669	THR
1	A	677	GLU
1	A	738	ARG
1	A	748	LYS

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

Mol	Chain	Res	Type
1	A	35	GLN
1	A	48	GLN
1	A	101	ASN
1	A	116	ASN
1	A	139	ASN
1	A	217	GLN
1	A	220	GLN
1	A	339	ASN
1	A	380	ASN

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Mol	Chain	Res	Type
1	A	415	ASN
1	A	442	GLN
1	A	478	GLN
1	A	512	ASN
1	A	516	GLN
1	A	547	GLN
1	A	574	GLN
1	A	582	GLN
1	A	603	GLN
1	A	635	ASN
1	A	639	GLN
1	A	643	GLN
1	A	749	ASN
1	A	760	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	HCS	A	772	-	6,7,7	0.86	0	5,8,8	1.03	0
3	SO4	A	771	-	4,4,4	0.40	0	6,6,6	0.07	0
5	THG	A	773	-	32,34,34	2.58	11 (34%)	39,47,47	2.28	9 (23%)
3	SO4	A	769	-	4,4,4	0.40	0	6,6,6	0.08	0
3	SO4	A	768	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	A	770	-	4,4,4	0.36	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
5	THG	A	773	-	1/1/5/9	10/22/31/31	0/3/3/3
4	HCS	A	772	-	-	1/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	773	THG	C6-N5	7.86	1.56	1.47
5	A	773	THG	O4-C4	7.53	1.37	1.23
5	A	773	THG	C9-N10	4.62	1.53	1.45
5	A	773	THG	C3'-C4'	3.08	1.44	1.39
5	A	773	THG	C5'-C6'	3.00	1.43	1.38
5	A	773	THG	C4A-N5	2.42	1.43	1.37
5	A	773	THG	C4A-C8A	2.40	1.42	1.38
5	A	773	THG	C1'-C11	2.37	1.55	1.50
5	A	773	THG	C2'-C3'	2.26	1.42	1.38
5	A	773	THG	C6'-C1'	2.24	1.42	1.39
5	A	773	THG	C2'-C1'	2.02	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	773	THG	C9-C6-N5	9.68	129.49	108.90
5	A	773	THG	C2-N1-C8A	4.56	121.41	113.36
5	A	773	THG	C6-C7-N8	3.87	117.64	110.60
5	A	773	THG	O4-C4-C4A	-3.19	119.58	127.26
5	A	773	THG	C4A-C4-N3	3.14	120.76	112.13
5	A	773	THG	C9-N10-C4'	2.52	128.41	122.00
5	A	773	THG	N3-C2-N1	-2.43	118.86	123.32
5	A	773	THG	N2-C2-N3	2.13	121.26	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	773	THG	OE1-CD-CG	-2.06	116.57	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	773	THG	C6

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	773	THG	N5-C6-C9-N10
5	A	773	THG	C2'-C1'-C11-O11
5	A	773	THG	C6'-C1'-C11-O11
5	A	773	THG	C2'-C1'-C11-N
5	A	773	THG	C6'-C1'-C11-N
4	A	772	HCS	CA-CB-CG-SD
5	A	773	THG	OX2-C-CA-N
5	A	773	THG	OX1-C-CA-N
5	A	773	THG	C6-C9-N10-C4'
5	A	773	THG	OE1-CD-CG-CB
5	A	773	THG	OE2-CD-CG-CB

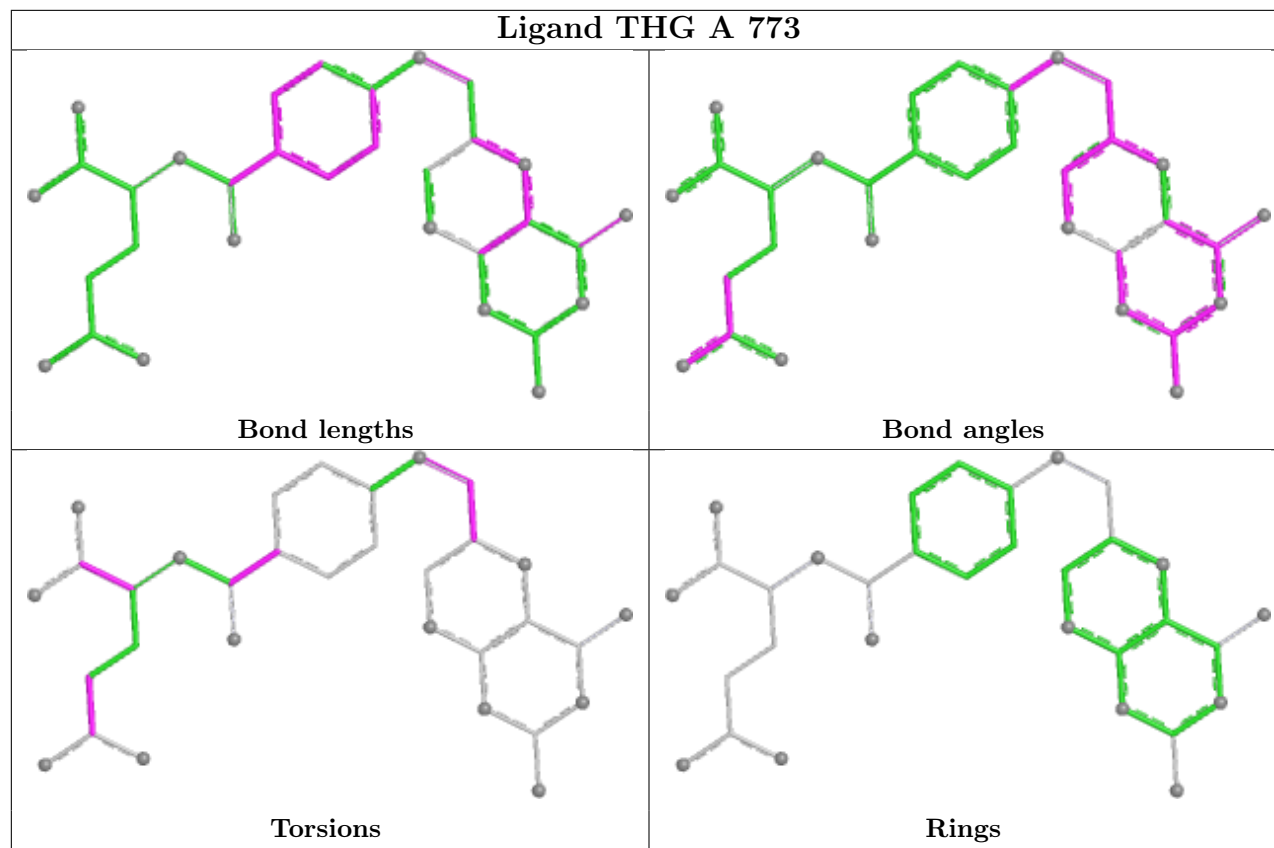
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	772	HCS	2	0
5	A	773	THG	1	0
3	A	769	SO4	2	0
3	A	768	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	728/765 (95%)	-1.40	0 100 100	22, 52, 83, 102	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

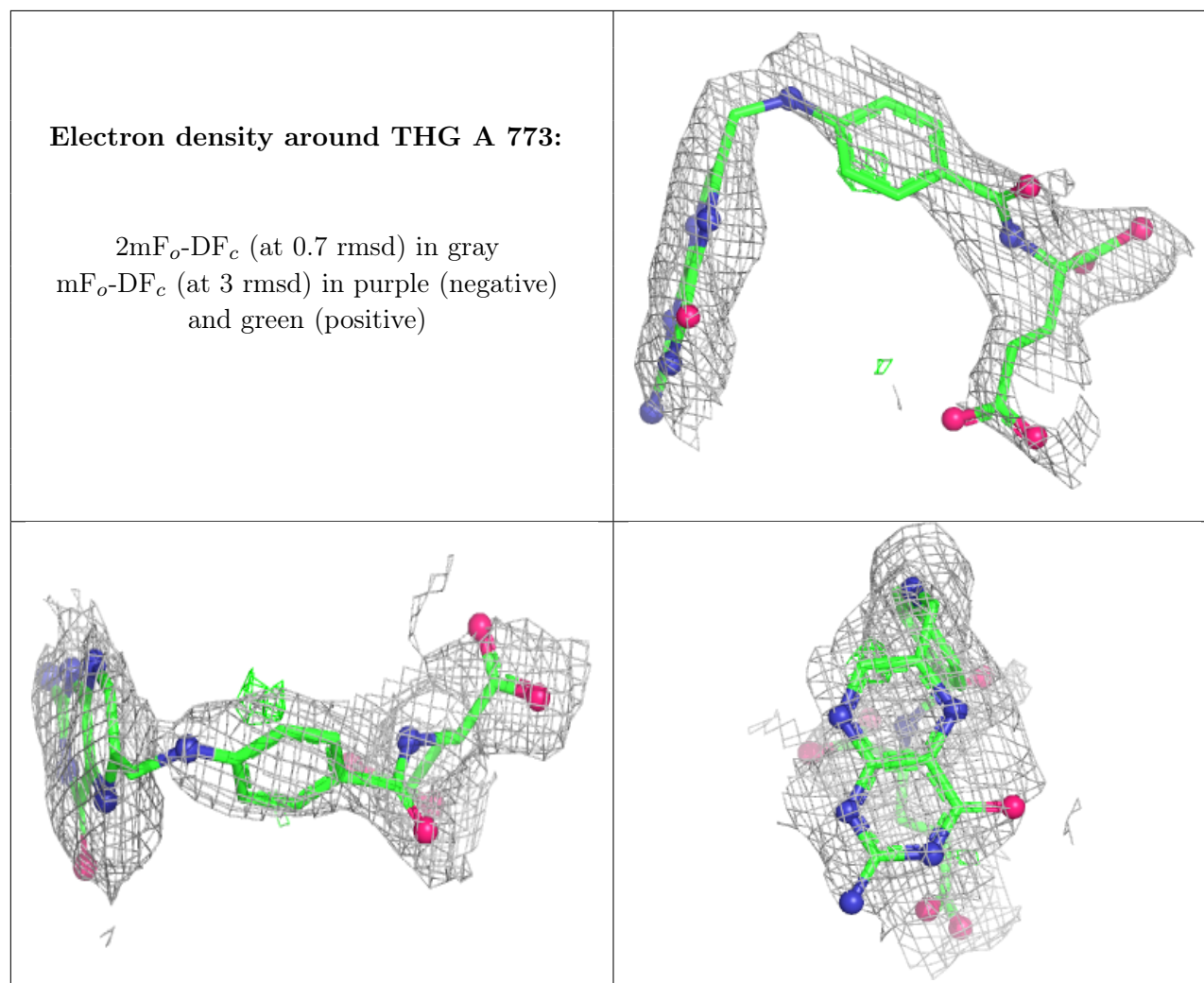
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	768	5/5	0.99	0.05	122,122,123,123	0
3	SO4	A	769	5/5	0.99	0.03	84,86,86,87	0
3	SO4	A	770	5/5	0.99	0.04	84,84,85,85	0
3	SO4	A	771	5/5	0.99	0.04	73,73,74,75	0
4	HCS	A	772	8/8	0.99	0.04	44,45,47,48	0
5	THG	A	773	32/32	0.99	0.06	64,72,80,82	0
2	ZN	A	766	1/1	1.00	0.01	62,62,62,62	0
2	ZN	A	767	1/1	1.00	0.01	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.