Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2024 – 10:40 AM EDT

PDB ID	:	1U22
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:

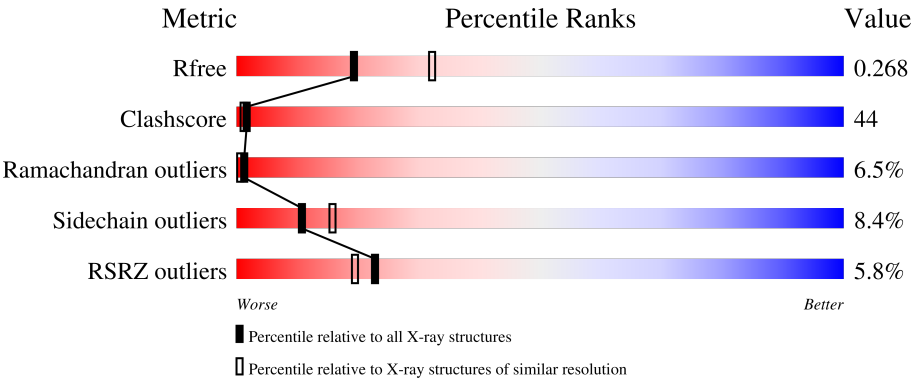
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	5% 37% 52% 8%

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 (i)

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
			Total	C	N	O	S	Se			
1	A	746	5783	3686	974	1099	6	18	0	0	0

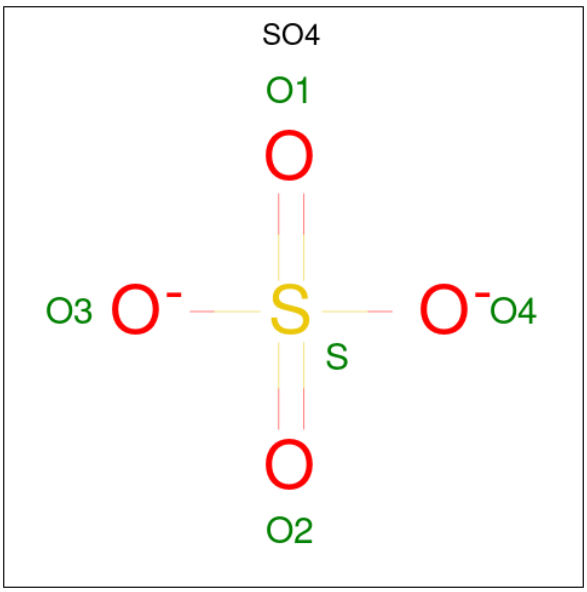
There are 19 discrepancies between the modelled and reference sequences:

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 (three-letter code: ZN) (formula: Zn).

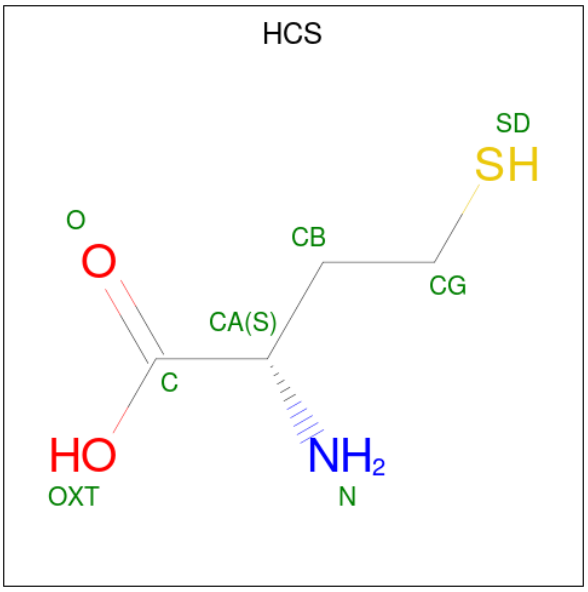
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



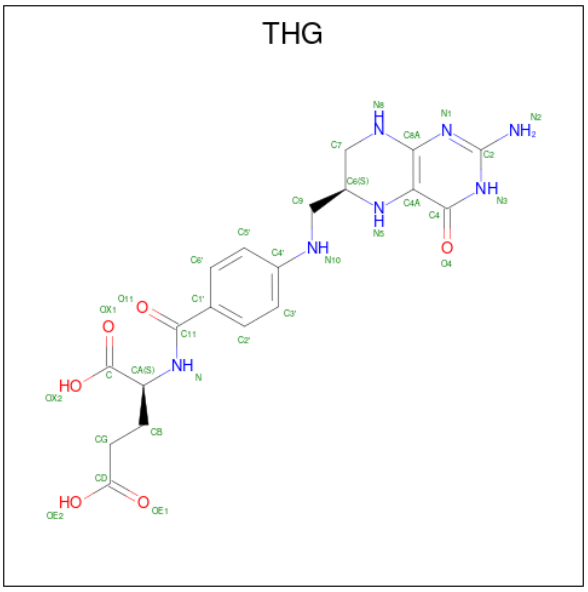
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: $C_4H_9NO_2S$).



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 (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).



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

- Molecule 6 is water.

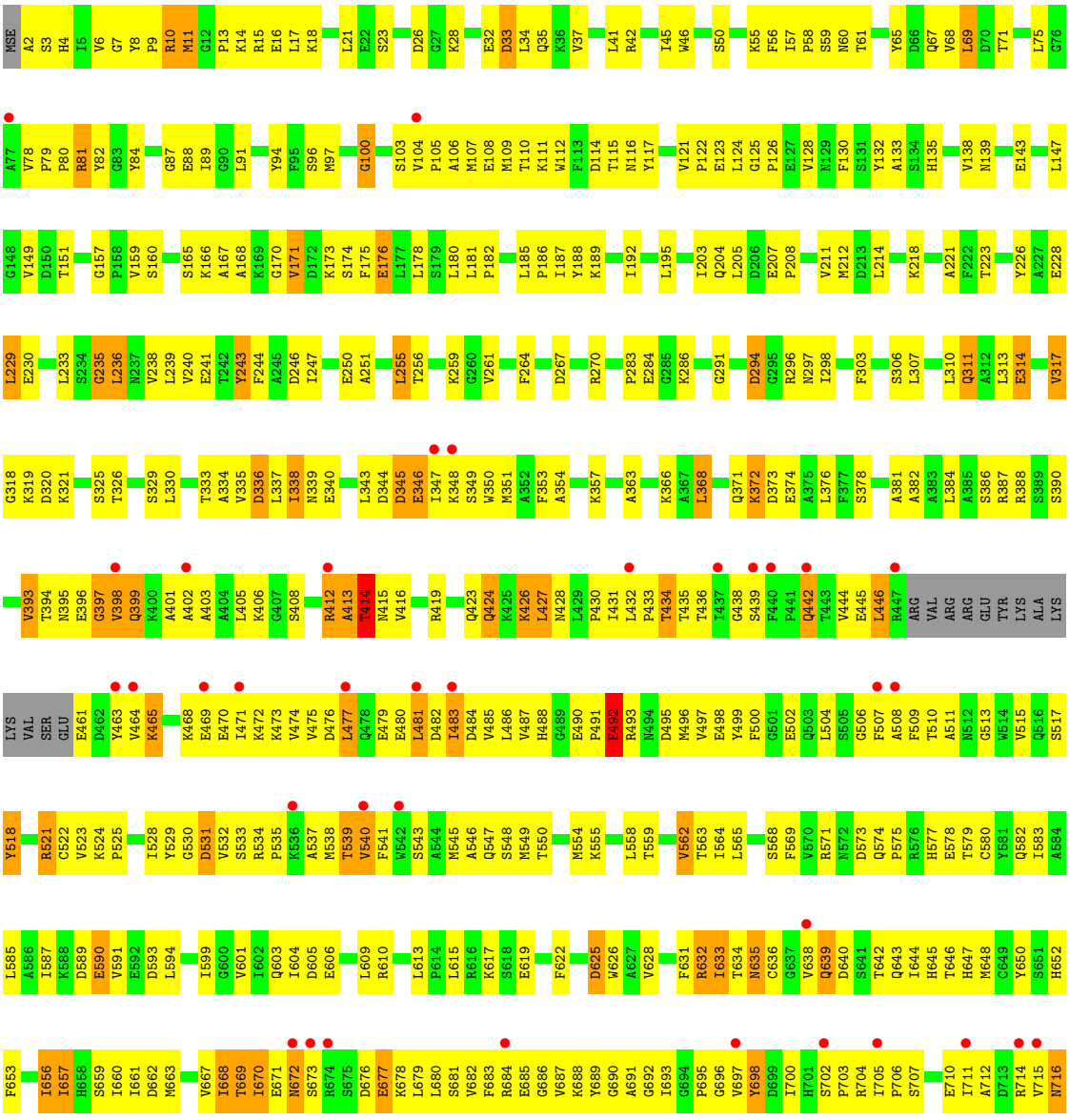
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	282	Total	O	0	0
			282	282		

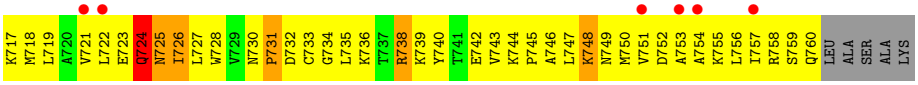
3 Residue-property plots (i)

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

Chain A:




K717
M718
L719
A720
V721
L722
E723
Q724
N725
I726
L727
W728
V729
N730
P731
D732
C733
G734
L735
K736
T737
R738
K739
Y740
T741
E742
V743
K744
P745
A746
L747
K748
N749
M750
V751
D752
A753
A754
K755
L756
I757
R758
S759
Q760
LEU
ALA
SER
ALA
LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.19 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.270 0.204 , 0.268	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 , 84.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.117 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HCS, ZN, THG, SO4

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	0.41	0/5884	0.66	1/7949 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	397	GLY	N-CA-C	-5.24	99.99	113.10

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	519	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	22	0
All	All	6127	0	5821	519	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 44.

All (519) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:157:GLY:HA3	1:A:207:GLU:CD	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:656:ILE:O	1:A:656:ILE:HG12	1.97	0.65
1:A:464:VAL:HG13	1:A:465:LYS:HZ2	1.62	0.64
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: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:510:THR:O	1:A:524:LYS:NZ	2.25	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: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: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: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: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:507:PHE:C	1:A:529:TYR:HE2	2.06	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:336:ASP:CG	1:A:338:ILE:HG22	2.24	0.58
1:A:756:LEU:HD12	1:A:760:GLN:HE22	1.69	0.58
1:A:685:GLU:C	1:A:687:VAL:H	2.07	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:318:GLY:C	1:A:320:ASP:H	2.07	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:397:GLY:C	1:A:399:GLN:H	2.08	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: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:413:ALA:O	1:A:414:THR:C	2.44	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: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:464:VAL:CG1	1:A:465:LYS:HZ2	2.22	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:685:GLU:C	1:A:687:VAL:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:OD1	1:A:338:ILE:HG22	2.08	0.52
1:A:696:GLY:CA	1:A:731:PRO:O	2.57	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:310:LEU:HB3	1:A:368:LEU:HD11	1.91	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:399:GLN:C	1:A:401:ALA:H	2.13	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:498:GLU:O	1:A:499:TYR:C	2.49	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: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:688:LYS:O	1:A:688:LYS:HG2	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: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: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: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: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:104:VAL:HG13	1:A:105:PRO:HD2	1.96	0.48
1:A:538:MSE:H	1:A:590:GLU:CD	2.17	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:401:ALA:C	1:A:403:ALA:H	2.16	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:726:ILE:HD12	1:A:726:ILE:C	2.35	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: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:508:ALA:N	1:A:529:TYR:HE2	2.14	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:399:GLN:C	1:A:399:GLN:CD	2.74	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:474:VAL:C	1:A:476:ASP:N	2.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:533:SER:C	1:A:535:PRO:HD3	2.37	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:170:GLY:O	1:A:171:VAL:C	2.55	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:283:PRO:HB2	1:A:286:LYS:CG	2.47	0.45
1:A:399:GLN:C	1:A:401:ALA:N	2.70	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HG13	1:A:353:PHE:CE1	2.53	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: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:702:SER:O	1:A:703:PRO:C	2.57	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:617:LYS:C	1:A:619:GLU:H	2.20	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: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: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:723:GLU:O	1:A:724:GLN:C	2.57	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
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:343:LEU:CB	1:A:348:LYS:CE	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:748:LYS:HB2	1:A:748:LYS:HZ2	1.85	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:112:TRP:HB3	1:A:115:THR:HG1	1.85	0.41
1:A:160:SER:OG	1:A:207:GLU:HA	2.21	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
1:A:401:ALA:O	1:A:405:LEU:CD2	2.68	0.40
1:A:493:ARG:NH2	1:A:539:THR:HG23	2.37	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: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 (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	742/765 (97%)	581 (78%)	113 (15%)	48 (6%)	1 0

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
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

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Mol	Chain	Res	Type
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 (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	622/619 (100%)	570 (92%)	52 (8%)	11 16

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
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	132	TYR
1	A	159	VAL
1	A	176	GLU
1	A	178	LEU
1	A	195	LEU
1	A	214	LEU
1	A	229	LEU
1	A	243	TYR
1	A	246	ASP

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Mol	Chain	Res	Type
1	A	255	LEU
1	A	311	GLN
1	A	314	GLU
1	A	336	ASP
1	A	345	ASP
1	A	368	LEU
1	A	399	GLN
1	A	414	THR
1	A	415	ASN
1	A	424	GLN
1	A	426	LYS
1	A	427	LEU
1	A	434	THR
1	A	436	THR
1	A	442	GLN
1	A	446	LEU
1	A	465	LYS
1	A	477	LEU
1	A	492	GLU
1	A	521	ARG
1	A	531	ASP
1	A	562	VAL
1	A	593	ASP
1	A	632	ARG
1	A	635	ASN
1	A	636	CYS
1	A	657	ILE
1	A	662	ASP
1	A	668	ILE
1	A	669	THR
1	A	677	GLU
1	A	684	ARG
1	A	716	ASN
1	A	724	GLN
1	A	738	ARG
1	A	748	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	220	GLN
1	A	339	ASN
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	716	ASN
1	A	760	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	SO4	A	769	-	4,4,4	0.29	0	6,6,6	0.13	0
5	THG	A	773	-	32,34,34	2.40	12 (37%)	39,47,47	2.29	9 (23%)
3	SO4	A	768	-	4,4,4	0.27	0	6,6,6	0.12	0
4	HCS	A	772	-	6,7,7	0.83	0	7,8,8	1.12	0
3	SO4	A	770	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	A	771	-	4,4,4	0.29	0	6,6,6	0.13	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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	773	THG	C6-N5	7.59	1.56	1.46
5	A	773	THG	O4-C4	5.29	1.37	1.24
5	A	773	THG	C9-N10	4.09	1.53	1.45
5	A	773	THG	C4-N3	3.67	1.39	1.33
5	A	773	THG	C3'-C4'	3.08	1.44	1.39
5	A	773	THG	C4A-N5	2.70	1.43	1.38
5	A	773	THG	C5'-C6'	2.70	1.43	1.38
5	A	773	THG	C1'-C11	2.50	1.55	1.50
5	A	773	THG	C8A-N1	2.15	1.38	1.34
5	A	773	THG	C6'-C1'	2.05	1.42	1.39
5	A	773	THG	C2'-C3'	2.04	1.42	1.38
5	A	773	THG	C5'-C4'	2.00	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	773	THG	C9-C6-N5	9.60	129.49	108.83
5	A	773	THG	N1-C2-N3	-4.18	118.86	125.42
5	A	773	THG	C6-C7-N8	3.71	117.64	110.68
5	A	773	THG	C2-N3-C4	3.69	121.79	115.93
5	A	773	THG	C2-N1-C8A	3.06	121.41	114.54
5	A	773	THG	C4-C4A-N5	2.74	121.42	119.12
5	A	773	THG	N2-C2-N3	2.58	121.26	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	773	THG	C9-N10-C4'	2.42	128.41	122.14
5	A	773	THG	OE1-CD-CG	-2.03	116.57	123.08

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
4	A	772	HCS	CA-CB-CG-SD
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
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

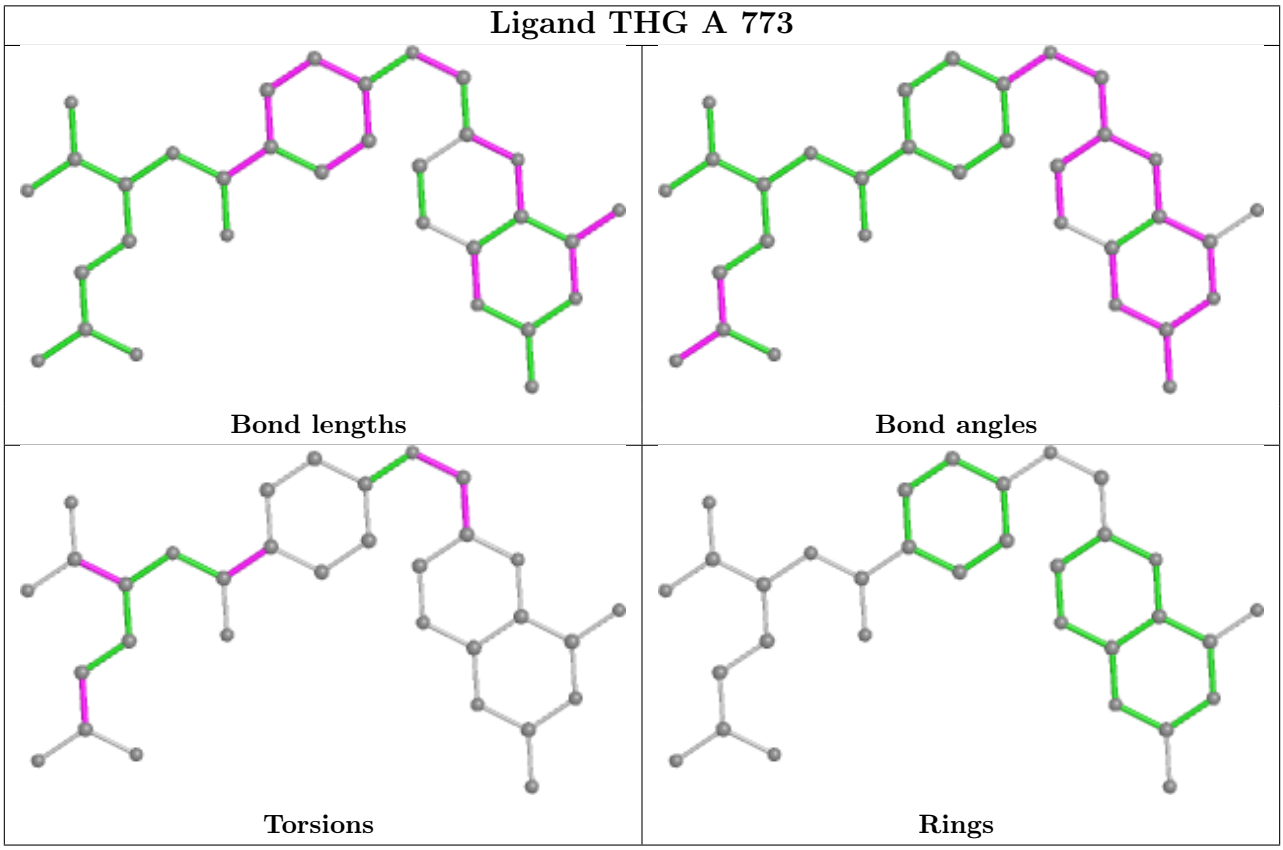
There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

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	728/765 (95%)	0.42	42 (5%)	23	19	22, 52, 83, 102	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	LEU	7.1
1	A	754	ALA	4.6
1	A	757	ILE	4.5
1	A	347	ILE	4.0
1	A	464	VAL	3.9
1	A	715	VAL	3.8
1	A	440	PHE	3.5
1	A	672	ASN	3.3
1	A	753	ALA	3.3
1	A	439	SER	3.2
1	A	471	ILE	3.2
1	A	721	VAL	3.0
1	A	463	TYR	2.9
1	A	542	TRP	2.8
1	A	540	VAL	2.8
1	A	432	LEU	2.8
1	A	705	ILE	2.7
1	A	702	SER	2.7
1	A	697	VAL	2.7
1	A	722	LEU	2.7
1	A	638	VAL	2.7
1	A	483	ILE	2.6
1	A	477	LEU	2.6
1	A	447	ARG	2.5
1	A	412	ARG	2.5
1	A	751	VAL	2.5
1	A	684	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	673	SER	2.3
1	A	674	ARG	2.3
1	A	442	GLN	2.3
1	A	104	VAL	2.3
1	A	714	ARG	2.3
1	A	469	GLU	2.2
1	A	437	ILE	2.2
1	A	507	PHE	2.2
1	A	398	VAL	2.2
1	A	508	ALA	2.2
1	A	402	ALA	2.2
1	A	711	ILE	2.1
1	A	77	ALA	2.1
1	A	536	LYS	2.0
1	A	348	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

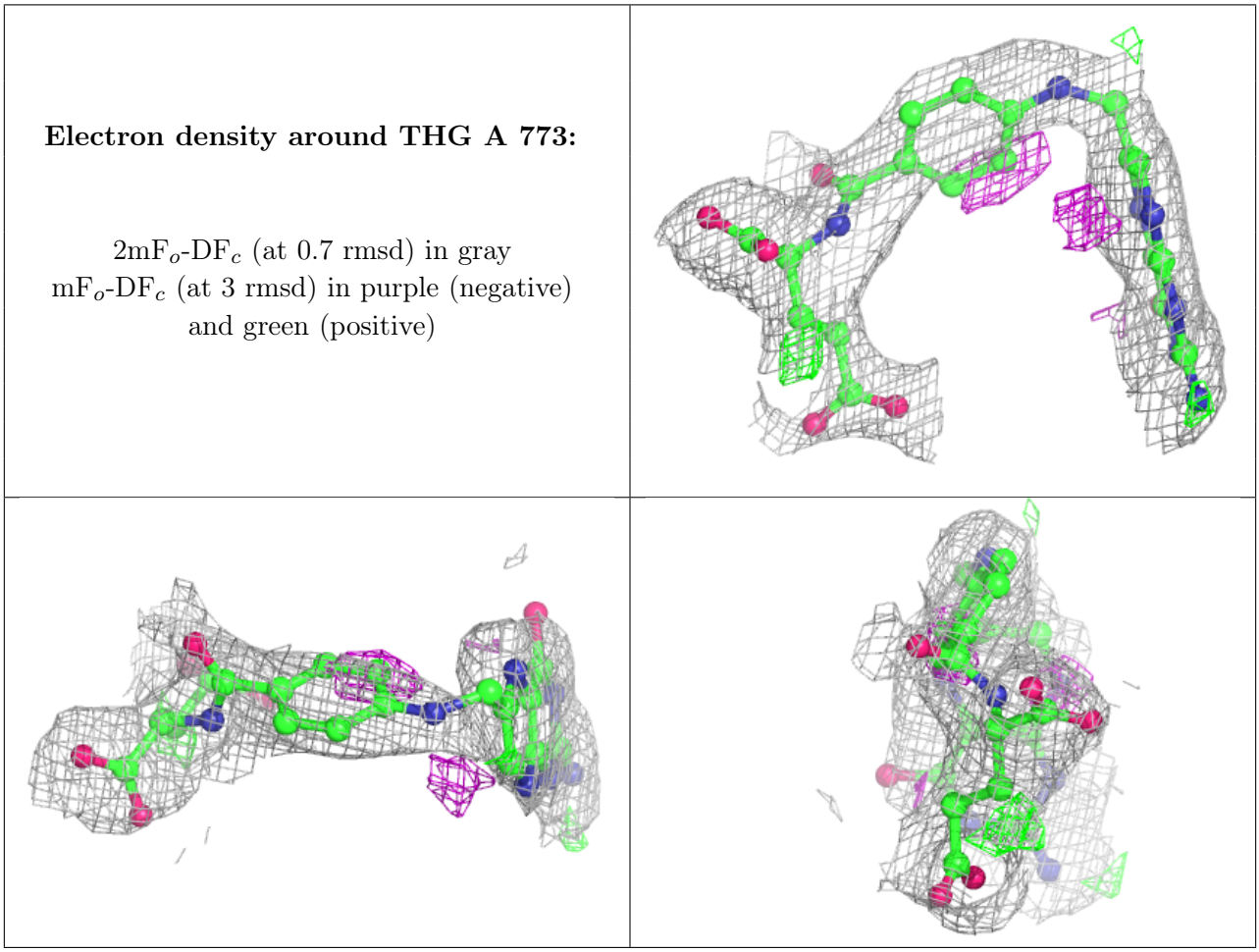
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	THG	A	773	32/32	0.73	0.29	64,72,80,82	0
3	SO4	A	769	5/5	0.89	0.15	84,86,86,87	0
3	SO4	A	768	5/5	0.89	0.27	122,122,123,123	0
4	HCS	A	772	8/8	0.91	0.25	44,45,47,48	0
3	SO4	A	771	5/5	0.96	0.17	73,73,74,75	0
3	SO4	A	770	5/5	0.97	0.18	84,84,85,85	0
2	ZN	A	766	1/1	0.99	0.15	62,62,62,62	0
2	ZN	A	767	1/1	1.00	0.19	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.

Electron density around THG A 773:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.