



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:12 am GMT

PDB ID : 3VE1
Title : The 2.9 angstrom crystal structure of Transferrin binding protein B (TbpB) from serogroup B M982 *Neisseria meningitidis* in complex with human transferrin
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2012-01-06
Resolution : 2.96 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

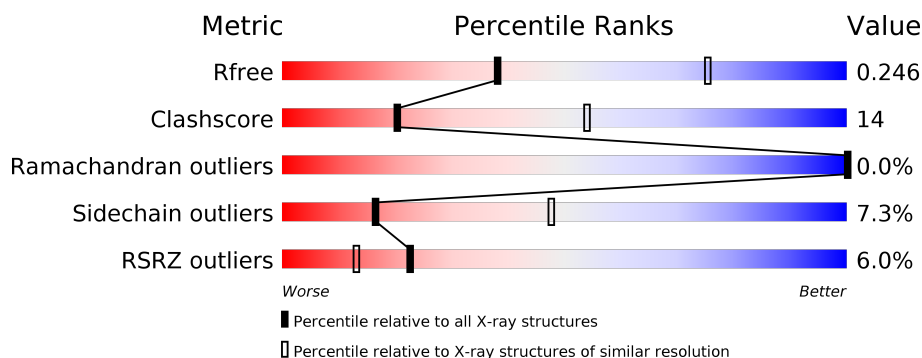
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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 $\leq 5\%$. 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	658	<div> <div>9%</div> <div> <div></div> <div>57%</div> <div>22%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	658	<div> <div>7%</div> <div> <div></div> <div>57%</div> <div>21%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	679	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>••</div> </div> </div>
2	D	679	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>•</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	703	-	-	-	X
3	GOL	B	704	-	-	X	-
3	GOL	B	705	-	-	-	X
3	GOL	B	707	-	-	-	X
3	GOL	B	708	-	-	-	X
3	GOL	C	701	-	-	-	X
3	GOL	D	703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19274 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 Transferrin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	1	0
			4240	2657	732	844	7			
1	C	536	Total	C	N	O	S	0	0	0
			4215	2640	726	842	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP Q09057
A	35	SER	-	EXPRESSION TAG	UNP Q09057
C	34	GLY	-	EXPRESSION TAG	UNP Q09057
C	35	SER	-	EXPRESSION TAG	UNP Q09057

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	675	Total	C	N	O	S	0	2	0
			5254	3296	910	1001	47			
2	D	677	Total	C	N	O	S	0	3	0
			5274	3310	913	1004	47			

There are 6 discrepancies between the modelled and reference sequences:

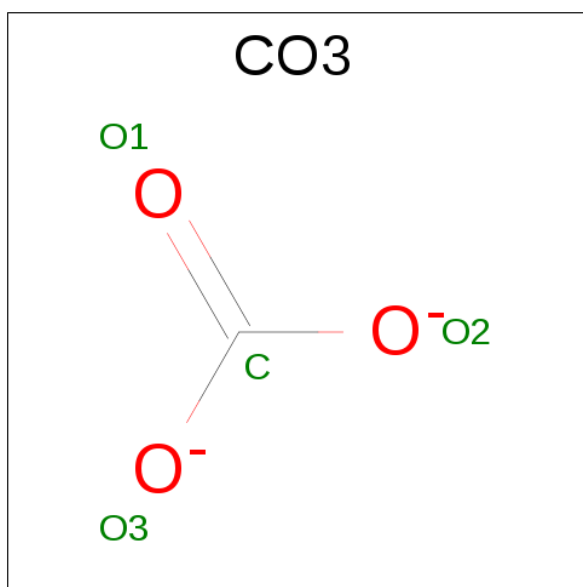
Chain	Residue	Modelled	Actual	Comment	Reference
B	413	ASP	ASN	SEE REMARK 999	UNP P02787
B	429	VAL	ILE	SEE REMARK 999	UNP P02787
B	611	ASP	ASN	SEE REMARK 999	UNP P02787
D	413	ASP	ASN	SEE REMARK 999	UNP P02787
D	429	VAL	ILE	SEE REMARK 999	UNP P02787
D	611	ASP	ASN	SEE REMARK 999	UNP P02787

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		
4	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

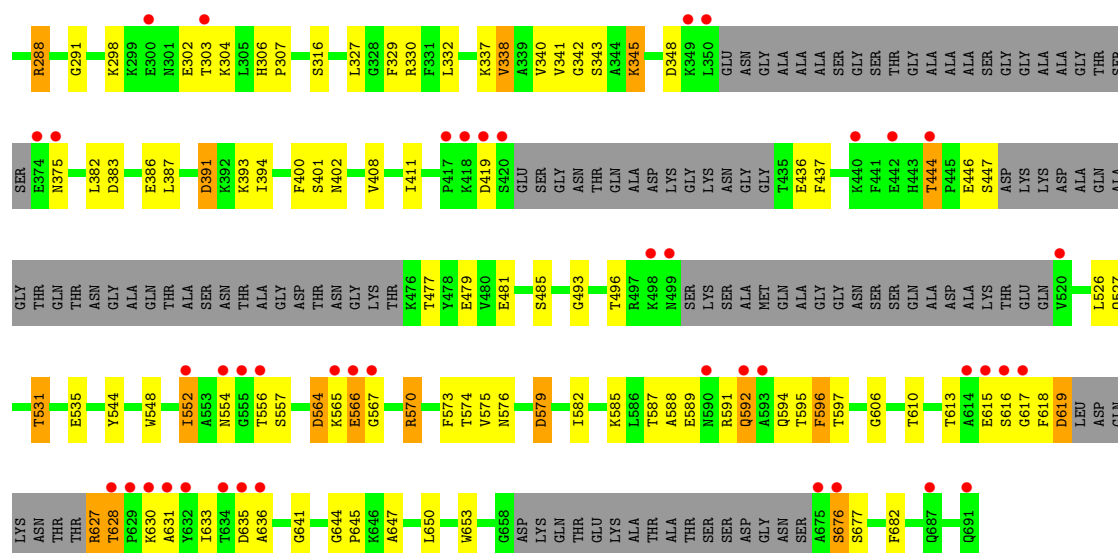
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		

- Molecule 6 is water.

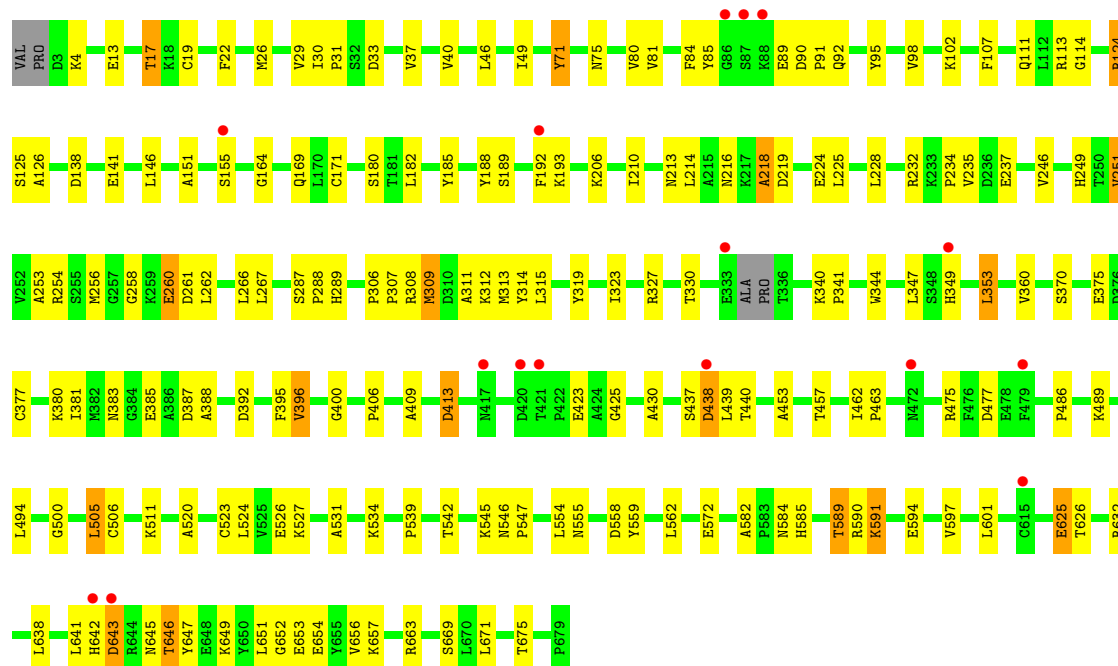
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	65	Total	O	0	0
			65	65		
6	C	34	Total	O	0	0
			34	34		
6	D	67	Total	O	0	0
			67	67		

- Molecule 1: Transferrin-binding protein 2

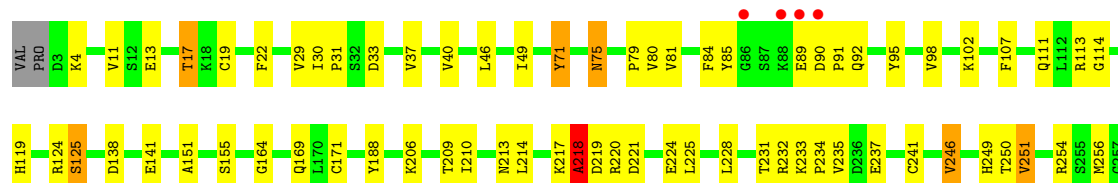
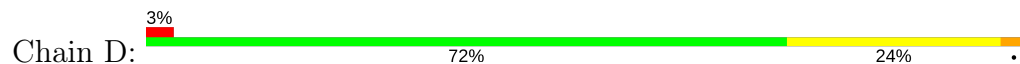


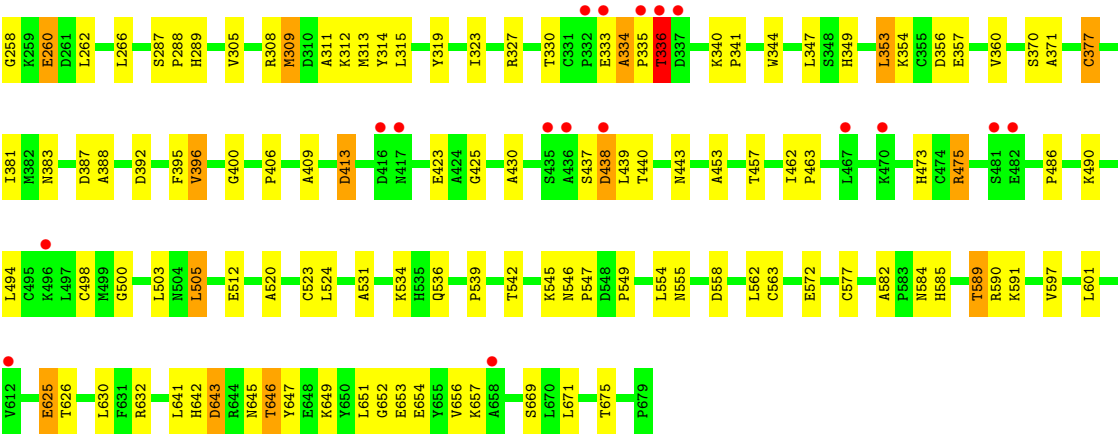


• Molecule 2: Serotransferrin



• Molecule 2: Serotransferrin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.02Å 153.51Å 169.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 2.96 38.12 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.93-2.96) 99.6 (38.12-2.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.95Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.249 0.202 , 0.246	Depositor DCC
R_{free} test set	2496 reflections (3.56%)	DCC
Wilson B-factor (Å ²)	56.8	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19274	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2640e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, CO3, FE

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	0.51	0/4331	0.71	4/5826 (0.1%)
1	C	0.52	0/4300	0.72	7/5782 (0.1%)
2	B	0.56	0/5375	0.68	1/7262 (0.0%)
2	D	0.57	0/5397	0.68	3/7295 (0.0%)
All	All	0.54	0/19403	0.69	15/26165 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	D	0	2
All	All	0	6

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	ARG	NE-CZ-NH2	-13.99	113.30	120.30
1	A	288	ARG	NE-CZ-NH1	-12.57	114.01	120.30
1	C	288	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	A	288	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	C	628	THR	C-N-CD	-9.48	99.74	120.60
2	B	218	ALA	N-CA-C	-7.42	90.95	111.00
1	C	628	THR	C-N-CA	6.69	150.09	122.00
1	C	288	ARG	CD-NE-CZ	6.23	132.33	123.60
1	A	288	ARG	CD-NE-CZ	5.97	131.96	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	218	ALA	N-CA-C	5.87	126.86	111.00
1	A	264	LEU	CA-CB-CG	5.49	127.94	115.30
2	D	334	ALA	N-CA-C	-5.40	96.42	111.00
1	C	264	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	298	LYS	N-CA-C	-5.31	96.67	111.00
2	D	383	ASN	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	SER	Peptide
1	A	564	ASP	Mainchain
1	C	108	SER	Peptide
1	C	564	ASP	Mainchain
2	D	218	ALA	Peptide
2	D	336	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4240	0	4066	133	0
1	C	4215	0	4040	127	0
2	B	5254	0	5065	136	0
2	D	5274	0	5088	139	0
3	A	12	0	16	2	0
3	B	36	0	48	8	0
3	C	6	0	8	3	0
3	D	24	0	32	5	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	37	0	0	3	0
6	B	65	0	0	8	0
6	C	34	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	67	0	0	4	0
All	All	19274	0	18363	525	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 14.

All (525) 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:B:218:ALA:O	2:B:219:ASP:HB2	1.49	1.11
2:B:124:ARG:HB3	3:B:704:GOL:H11	1.37	1.06
2:D:49:ILE:HG22	2:D:75:ASN:HD22	1.23	1.04
1:C:587:THR:HG21	1:C:592:GLN:NE2	1.80	0.96
1:C:288:ARG:HD3	3:C:701:GOL:H32	1.45	0.96
1:C:587:THR:CG2	1:C:592:GLN:HE21	1.79	0.96
2:B:49:ILE:HG22	2:B:75:ASN:HD22	1.31	0.95
1:A:206:LYS:HE3	6:B:801:HOH:O	1.64	0.94
2:B:388:ALA:HB2	2:B:589:THR:HG23	1.51	0.92
1:C:206:LYS:HE3	6:D:849:HOH:O	1.71	0.91
1:A:556:THR:HG22	1:A:620:LEU:HG	1.54	0.89
1:A:554:ASN:HB2	1:A:676:SER:OG	1.74	0.87
1:C:587:THR:CG2	1:C:592:GLN:NE2	2.38	0.87
2:D:234:PRO:HD2	2:D:237:GLU:HG3	1.58	0.86
1:C:627:ARG:HD3	1:C:628:THR:HG23	1.57	0.86
2:B:234:PRO:HD2	2:B:237:GLU:HG3	1.59	0.84
2:D:388:ALA:HB2	2:D:589:THR:HG23	1.58	0.84
1:A:587:THR:HG21	1:A:592:GLN:NE2	1.93	0.83
1:C:554:ASN:HB2	1:C:676:SER:OG	1.79	0.83
2:B:4:LYS:HB2	2:B:262:LEU:HD21	1.61	0.82
2:D:210[A]:ILE:HD13	2:D:235:VAL:HG11	1.62	0.82
2:B:646:THR:HG23	2:B:649:LYS:HD2	1.62	0.81
2:D:646:THR:HG23	2:D:649:LYS:HD2	1.61	0.80
1:A:567:GLY:O	1:A:589:GLU:HA	1.82	0.79
2:B:288:PRO:HG2	2:B:289:HIS:HD2	1.48	0.79
1:A:479:GLU:HB3	1:A:496:THR:HG22	1.66	0.78
1:C:52:TRP:HA	1:C:57:GLU:HG3	1.66	0.78
2:B:643:ASP:OD1	2:B:643:ASP:N	2.14	0.78
1:C:567:GLY:O	1:C:589:GLU:HA	1.83	0.78
1:C:565:LYS:HB2	1:C:566:GLU:HA	1.66	0.77
2:D:643:ASP:OD1	2:D:643:ASP:N	2.18	0.77
1:A:594:GLN:HG2	1:A:619:ASP:OD2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:GLU:HB3	1:C:496:THR:HG22	1.66	0.76
1:C:594:GLN:HG2	1:C:619:ASP:OD2	1.84	0.76
2:D:188:TYR:CZ	3:D:703:GOL:H32	2.21	0.76
2:B:288:PRO:HG2	2:B:289:HIS:CD2	2.21	0.76
2:D:13:GLU:O	2:D:17:THR:HG22	1.86	0.76
1:C:479:GLU:HB3	1:C:496:THR:CG2	2.16	0.75
1:A:52:TRP:HA	1:A:57:GLU:HG3	1.67	0.75
1:C:564:ASP:O	1:C:565:LYS:HG2	1.86	0.75
1:A:529:GLU:HB3	3:A:702:GOL:H32	1.68	0.75
2:D:210[A]:ILE:CD1	2:D:235:VAL:HG11	2.16	0.75
1:C:266:ASN:O	1:C:267:ASN:HB2	1.85	0.74
1:A:587:THR:CG2	1:A:592:GLN:HE21	2.00	0.74
1:A:266:ASN:O	1:A:267:ASN:HB2	1.86	0.74
1:A:479:GLU:HB3	1:A:496:THR:CG2	2.17	0.73
2:B:589:THR:HG21	2:B:597:VAL:HG21	1.69	0.73
1:C:288:ARG:CD	3:C:701:GOL:H32	2.19	0.73
1:A:265:ASN:HB2	2:B:526:GLU:O	1.87	0.73
1:A:587:THR:CG2	1:A:592:GLN:NE2	2.51	0.73
1:C:226:LYS:HG3	1:C:227:ASN:HD22	1.53	0.73
1:A:306:HIS:HB2	1:A:307:PRO:HD2	1.68	0.73
2:B:13:GLU:O	2:B:17:THR:HG22	1.89	0.73
1:C:616:SER:O	1:C:630:LYS:HD3	1.89	0.73
1:A:120:ASN:O	1:A:121:GLN:HB2	1.89	0.72
1:A:592:GLN:HB2	1:A:595:THR:HB	1.72	0.72
2:B:218:ALA:O	2:B:219:ASP:CB	2.28	0.72
2:D:210[B]:ILE:H	2:D:210[B]:ILE:HD12	1.54	0.71
1:A:616:SER:O	1:A:630:LYS:HD3	1.91	0.71
2:D:392:ASP:HA	2:D:585:HIS:CD2	2.24	0.71
1:A:300:GLU:HA	1:A:302:GLU:N	2.05	0.70
1:A:444:THR:HG23	1:A:477:THR:HG23	1.73	0.70
1:A:49:ARG:HB3	1:A:156:LYS:HB3	1.72	0.70
1:A:556:THR:O	1:A:620:LEU:HD11	1.91	0.70
2:D:218:ALA:HA	2:D:221:ASP:HB2	1.74	0.70
2:D:288:PRO:HG2	2:D:289:HIS:CD2	2.27	0.70
2:D:49:ILE:HG22	2:D:75:ASN:ND2	2.05	0.69
1:C:120:ASN:ND2	1:C:120:ASN:O	2.19	0.69
2:D:413:ASP:HB2	2:D:423:GLU:OE2	1.93	0.69
1:C:306:HIS:HB2	1:C:307:PRO:HD2	1.75	0.69
1:C:592:GLN:HA	1:C:594:GLN:H	1.59	0.68
2:B:81:VAL:HB	2:B:251:VAL:CG1	2.23	0.68
2:B:392:ASP:HA	2:B:585:HIS:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:HB3	1:C:156:LYS:HB3	1.75	0.68
2:D:288:PRO:HG2	2:D:289:HIS:HD2	1.58	0.68
1:C:124:ASN:HD21	1:C:185:VAL:HB	1.59	0.67
2:D:589:THR:HG21	2:D:597:VAL:HG21	1.76	0.67
1:A:120:ASN:HB2	1:A:121:GLN:OE1	1.95	0.67
1:A:226:LYS:HG3	1:A:227:ASN:HD22	1.60	0.67
2:D:4:LYS:HB2	2:D:262:LEU:HD21	1.75	0.67
2:D:188:TYR:OH	3:D:703:GOL:H32	1.95	0.67
1:A:197:ASP:OD1	1:A:199:ARG:HG3	1.96	0.66
1:C:124:ASN:ND2	1:C:185:VAL:HG11	2.10	0.66
2:B:81:VAL:HB	2:B:251:VAL:HG13	1.77	0.66
2:D:81:VAL:HB	2:D:251:VAL:CG1	2.25	0.66
1:C:226:LYS:HG3	1:C:227:ASN:ND2	2.11	0.66
1:A:613:THR:HG23	1:A:633:ILE:HB	1.78	0.65
1:C:592:GLN:HB2	1:C:595:THR:HB	1.78	0.65
1:C:444:THR:HG23	1:C:477:THR:HG23	1.78	0.65
2:D:387:ASP:O	2:D:589:THR:HG22	1.97	0.65
1:A:565:LYS:HB2	1:A:566:GLU:HA	1.79	0.65
1:A:227:ASN:HD22	1:A:227:ASN:N	1.93	0.65
2:D:217:LYS:O	2:D:218:ALA:HB3	1.97	0.64
1:C:124:ASN:ND2	1:C:185:VAL:CG1	2.60	0.64
1:C:391:ASP:OD1	1:C:391:ASP:N	2.30	0.64
2:D:218:ALA:HA	2:D:221:ASP:CB	2.28	0.64
1:A:226:LYS:HG3	1:A:227:ASN:ND2	2.13	0.63
1:C:197:ASP:OD1	1:C:199:ARG:HG3	1.98	0.63
2:D:71:TYR:OH	2:D:312:LYS:HE3	1.98	0.63
2:D:209:THR:O	2:D:213[A]:ASN:ND2	2.30	0.63
2:B:253:ALA:HB1	6:B:856:HOH:O	1.99	0.63
1:C:253:LEU:HG	1:C:282:ALA:HB3	1.80	0.63
2:D:457:THR:HG21	2:D:582:ALA:HB1	1.79	0.63
2:B:387:ASP:O	2:B:589:THR:HG22	1.98	0.62
1:C:587:THR:HG22	1:C:592:GLN:HE21	1.62	0.62
1:A:124:ASN:ND2	1:A:185:VAL:CG1	2.63	0.62
2:D:81:VAL:HB	2:D:251:VAL:HG13	1.81	0.62
1:C:588:ALA:HB3	1:C:594:GLN:HB3	1.82	0.62
2:D:430:ALA:HB3	2:D:562:LEU:HB2	1.82	0.61
1:C:613:THR:HG23	1:C:633:ILE:HB	1.81	0.61
2:B:375:GLU:OE2	3:B:707:GOL:H32	2.00	0.61
2:D:406:PRO:HD2	2:D:645:ASN:O	2.00	0.60
1:A:253:LEU:HG	1:A:282:ALA:HB3	1.82	0.60
1:A:576:ASN:CG	1:A:579:ASP:HB2	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:ARG:HB2	2:D:669:SER:HB3	1.83	0.60
1:A:53:TYR:CD1	1:A:153:LYS:HB3	2.37	0.60
2:B:406:PRO:HD2	2:B:645:ASN:O	2.00	0.60
2:B:323:ILE:HD11	2:B:327:ARG:NH2	2.17	0.60
1:A:206:LYS:CE	6:B:801:HOH:O	2.34	0.60
1:A:201:ILE:HG13	1:A:202:ILE:H	1.68	0.59
2:B:308:ARG:HB2	2:B:669:SER:HB3	1.84	0.59
2:D:323:ILE:HD11	2:D:327:ARG:NH2	2.18	0.59
1:C:587:THR:HG21	1:C:592:GLN:HE22	1.62	0.59
1:A:129:HIS:CD2	1:A:129:HIS:N	2.71	0.59
1:C:565:LYS:HB2	1:C:566:GLU:CA	2.32	0.59
2:B:71:TYR:OH	2:B:312:LYS:HE3	2.02	0.59
1:C:73:LEU:HD12	1:C:74:PRO:HD2	1.85	0.58
2:D:228:LEU:HB2	3:D:705:GOL:H32	1.85	0.58
2:D:327:ARG:HG2	2:D:327:ARG:HH11	1.68	0.58
1:C:155:ILE:HD12	2:D:360:VAL:HG21	1.84	0.58
1:C:146:SER:OG	2:D:356:ASP:OD2	2.22	0.58
2:B:413:ASP:HB2	2:B:423:GLU:OE2	2.03	0.58
2:D:19:CYS:O	2:D:22:PHE:HB3	2.03	0.58
1:C:227:ASN:HD22	1:C:227:ASN:N	2.01	0.58
2:B:31:PRO:HG3	1:C:133:GLN:HB3	1.86	0.57
1:A:391:ASP:N	1:A:391:ASP:OD1	2.33	0.57
2:D:457:THR:HG21	2:D:582:ALA:CB	2.33	0.57
2:D:319:TYR:O	2:D:323:ILE:HG22	2.05	0.57
1:C:53:TYR:CD1	1:C:153:LYS:HB3	2.39	0.57
1:C:201:ILE:HG13	1:C:202:ILE:H	1.68	0.57
1:C:345:LYS:HE3	1:C:348:ASP:OD1	2.05	0.57
2:B:319:TYR:O	2:B:323:ILE:HG22	2.05	0.57
2:D:652:GLY:O	2:D:656:VAL:HG13	2.05	0.56
2:B:327:ARG:HH11	2:B:327:ARG:HG2	1.70	0.56
2:B:84:PHE:CD1	2:B:91:PRO:HB3	2.40	0.56
2:B:192:PHE:CZ	2:B:210:ILE:HD12	2.40	0.56
1:C:124:ASN:HD22	1:C:185:VAL:HG11	1.68	0.56
2:D:231:THR:HB	6:D:820:HOH:O	2.06	0.56
1:A:529:GLU:CB	3:A:702:GOL:H32	2.36	0.56
2:B:671:LEU:O	2:B:675:THR:HG23	2.05	0.56
1:A:588:ALA:HB3	1:A:594:GLN:HB3	1.88	0.56
2:B:26:MET:HE1	2:B:30:ILE:HD11	1.88	0.56
1:A:124:ASN:HD22	1:A:124:ASN:C	2.10	0.55
1:A:345:LYS:HE3	1:A:348:ASP:OD1	2.06	0.55
2:B:256:MET:HA	2:B:256:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:ASN:CG	1:C:579:ASP:HB2	2.26	0.55
2:D:80:VAL:HG11	2:D:260:GLU:HG2	1.89	0.55
1:A:124:ASN:ND2	1:A:185:VAL:HG11	2.22	0.55
1:A:265:ASN:HD22	2:B:527:LYS:HA	1.72	0.55
2:B:224:GLU:OE1	2:B:232:ARG:HD3	2.07	0.55
1:A:382:LEU:C	1:A:382:LEU:HD12	2.28	0.55
1:C:565:LYS:HG3	1:C:566:GLU:HG2	1.87	0.54
2:D:542:THR:HG22	2:D:554:LEU:HB3	1.89	0.54
2:D:653:GLU:HG3	2:D:654:GLU:N	2.22	0.54
1:A:332:LEU:HD12	1:A:338:VAL:O	2.07	0.54
2:D:437:SER:O	2:D:438:ASP:HB3	2.08	0.54
2:B:49:ILE:HG22	2:B:75:ASN:ND2	2.13	0.54
2:B:85:TYR:HD2	2:B:92:GLN:O	1.91	0.54
2:B:542:THR:HG22	2:B:554:LEU:HB3	1.90	0.54
2:B:457:THR:HG21	2:B:582:ALA:HB1	1.90	0.54
2:D:4:LYS:HD3	2:D:262:LEU:HD11	1.90	0.54
2:D:344:TRP:CZ3	2:D:601:LEU:HD11	2.42	0.53
2:B:19:CYS:O	2:B:22:PHE:HB3	2.08	0.53
2:D:84:PHE:CD1	2:D:91:PRO:HB3	2.43	0.53
1:A:124:ASN:HD21	1:A:185:VAL:CG1	2.21	0.53
2:B:430:ALA:HB3	2:B:562:LEU:HB2	1.89	0.53
2:B:80:VAL:HG11	2:B:260:GLU:HG2	1.90	0.53
1:C:124:ASN:HD21	1:C:185:VAL:CG1	2.21	0.53
2:D:500:GLY:HA3	2:D:505:LEU:HA	1.90	0.53
1:C:129:HIS:CG	1:C:183:LYS:HB2	2.43	0.53
1:C:124:ASN:HD21	1:C:185:VAL:CB	2.20	0.53
1:C:617:GLY:HA3	1:C:630:LYS:HB3	1.91	0.53
2:B:124:ARG:HB3	3:B:704:GOL:C1	2.26	0.53
1:A:531:THR:HG21	1:A:647:ALA:HA	1.90	0.53
1:C:544:TYR:HB2	1:C:573:PHE:HB2	1.91	0.53
1:A:617:GLY:HA3	1:A:630:LYS:HB3	1.91	0.52
1:C:206:LYS:CE	6:D:849:HOH:O	2.43	0.52
2:B:71:TYR:HB2	2:B:311:ALA:CB	2.40	0.52
1:C:650:LEU:C	1:C:650:LEU:HD12	2.29	0.52
2:D:344:TRP:HZ3	2:D:601:LEU:HD11	1.73	0.52
2:B:653:GLU:O	2:B:657:LYS:HG3	2.09	0.52
2:D:333:GLU:N	2:D:334:ALA:HB2	2.24	0.52
2:B:126:ALA:N	3:B:704:GOL:H12	2.25	0.52
1:A:618:PHE:O	1:A:619:ASP:OD2	2.28	0.52
2:D:85:TYR:HD2	2:D:92:GLN:O	1.93	0.52
2:D:217:LYS:O	2:D:218:ALA:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HG13	1:C:202:ILE:N	2.25	0.51
1:A:201:ILE:HG13	1:A:202:ILE:N	2.25	0.51
1:A:544:TYR:HB2	1:A:573:PHE:HB2	1.91	0.51
2:B:437:SER:O	2:B:438:ASP:HB3	2.09	0.51
2:B:652:GLY:O	2:B:656:VAL:HG13	2.11	0.51
2:B:323:ILE:HD11	2:B:327:ARG:CZ	2.41	0.51
1:C:382:LEU:C	1:C:382:LEU:HD12	2.31	0.51
2:D:81:VAL:HB	2:D:251:VAL:HG11	1.93	0.51
2:B:254:ARG:HB2	2:B:258:GLY:HA2	1.93	0.51
2:B:287:SER:OG	2:B:288:PRO:HD2	2.11	0.51
1:C:592:GLN:HG2	1:C:592:GLN:O	2.11	0.51
2:D:71:TYR:HB2	2:D:311:ALA:CB	2.41	0.51
2:D:425:GLY:HA2	2:D:584:ASN:OD1	2.10	0.51
2:B:425:GLY:HA2	2:B:584:ASN:OD1	2.11	0.51
2:D:646:THR:CG2	2:D:649:LYS:HD2	2.37	0.50
1:A:592:GLN:HA	1:A:593:ALA:HB3	1.93	0.50
1:A:650:LEU:C	1:A:650:LEU:HD12	2.32	0.50
2:B:113:ARG:NH1	6:B:811:HOH:O	2.43	0.50
2:B:4:LYS:HD3	2:B:262:LEU:HD11	1.94	0.50
2:D:371:ALA:HB3	2:D:377:CYS:SG	2.51	0.50
1:C:531:THR:HG21	1:C:647:ALA:HA	1.93	0.50
1:C:575:VAL:HG22	1:C:582:ILE:HG13	1.93	0.50
2:D:462:ILE:HB	2:D:463:PRO:HD3	1.92	0.50
2:D:98:VAL:HB	2:D:225:LEU:HD22	1.93	0.50
1:A:554:ASN:HB2	1:A:676:SER:HG	1.75	0.50
2:B:81:VAL:HB	2:B:251:VAL:HG11	1.94	0.50
1:A:552:ILE:HD11	1:A:631:ALA:HB1	1.94	0.49
2:B:126:ALA:H	3:B:704:GOL:H12	1.77	0.49
1:C:244:LEU:HD12	1:C:244:LEU:N	2.26	0.49
1:C:332:LEU:HD12	1:C:338:VAL:O	2.12	0.49
2:B:396:VAL:HG22	2:B:651:LEU:HD21	1.94	0.49
1:C:264:LEU:CD2	1:C:264:LEU:N	2.75	0.49
2:D:233:LYS:HD2	2:D:241:CYS:HB2	1.93	0.49
2:D:653:GLU:O	2:D:657:LYS:HG3	2.12	0.49
2:D:125:SER:H	3:D:703:GOL:H2	1.77	0.49
1:A:345:LYS:CE	1:A:348:ASP:OD1	2.61	0.49
2:B:396:VAL:CG2	2:B:651:LEU:HD21	2.42	0.49
1:A:266:ASN:O	1:A:267:ASN:CB	2.60	0.49
1:C:93:THR:CG2	1:C:142:LYS:HD3	2.42	0.49
1:C:52:TRP:CH2	2:D:357:GLU:HA	2.48	0.49
2:D:520:ALA:O	2:D:523:CYS:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:LYS:NZ	2:B:594:GLU:OE2	2.32	0.49
1:C:585:LYS:HA	1:C:596:PHE:O	2.13	0.49
2:D:335:PRO:CB	2:D:336:THR:HG22	2.42	0.49
1:A:270:ASN:O	1:A:271:ASP:HB2	2.13	0.49
2:B:37:VAL:HG22	2:B:266:LEU:HD21	1.95	0.49
2:B:409:ALA:HB2	2:B:641:LEU:HD21	1.94	0.49
2:D:671:LEU:O	2:D:675:THR:HG23	2.12	0.49
1:C:266:ASN:O	1:C:267:ASN:CB	2.59	0.49
1:A:594:GLN:HB3	1:A:618:PHE:CZ	2.48	0.48
2:D:254:ARG:HB2	2:D:258:GLY:HA2	1.94	0.48
1:A:264:LEU:CD2	1:A:264:LEU:N	2.76	0.48
1:A:592:GLN:O	1:A:592:GLN:HG2	2.11	0.48
1:C:552:ILE:HD11	1:C:631:ALA:HB1	1.94	0.48
1:A:281:ASP:O	1:A:291:GLY:HA3	2.14	0.48
2:B:17:THR:HG21	6:B:844:HOH:O	2.13	0.48
1:A:93:THR:CG2	1:A:142:LYS:HD3	2.43	0.48
2:B:188:TYR:CZ	2:B:206:LYS:HD3	2.49	0.48
2:B:309:MET:HE2	2:B:313:MET:HG2	1.95	0.48
2:B:457:THR:HG21	2:B:582:ALA:CB	2.43	0.48
1:C:618:PHE:O	1:C:619:ASP:OD2	2.31	0.48
1:A:539:ASP:HB3	6:A:836:HOH:O	2.13	0.48
1:A:575:VAL:HG22	1:A:582:ILE:HG13	1.96	0.48
2:D:224:GLU:OE1	2:D:232:ARG:HD3	2.13	0.48
2:B:534:LYS:HD2	2:B:632:ARG:NH2	2.29	0.48
1:C:46:ARG:HB2	1:C:162:TYR:CE1	2.49	0.48
2:D:323:ILE:HD11	2:D:327:ARG:CZ	2.44	0.48
6:C:834:HOH:O	2:D:353:LEU:HD12	2.13	0.48
2:B:653:GLU:HG3	2:B:654:GLU:N	2.28	0.48
1:C:267:ASN:O	1:C:270:ASN:HB3	2.14	0.48
2:D:256:MET:HA	2:D:256:MET:HE3	1.95	0.48
1:A:120:ASN:CB	1:A:121:GLN:OE1	2.61	0.48
2:B:164:GLY:HA3	2:B:171:CYS:SG	2.53	0.48
2:B:234:PRO:CD	2:B:237:GLU:HG3	2.37	0.48
1:C:198:PHE:HB3	1:C:306:HIS:HA	1.96	0.48
2:D:462:ILE:HB	2:D:463:PRO:CD	2.44	0.48
2:D:453:ALA:HA	2:D:486:PRO:HD2	1.96	0.48
2:B:289:HIS:CD2	2:B:289:HIS:N	2.81	0.48
2:B:462:ILE:HB	2:B:463:PRO:HD3	1.96	0.48
1:A:198:PHE:HB3	1:A:306:HIS:HA	1.94	0.47
1:A:565:LYS:HG3	1:A:566:GLU:HG2	1.96	0.47
1:C:606:GLY:HA2	1:C:641:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:TRP:HB3	1:A:682:PHE:HB3	1.96	0.47
2:B:113:ARG:NH2	2:B:138:ASP:O	2.47	0.47
2:B:344:TRP:CZ3	2:B:601:LEU:HD11	2.49	0.47
1:A:519:GLN:HG2	1:A:520:VAL:HG23	1.96	0.47
2:B:601:LEU:HA	2:B:601:LEU:HD23	1.57	0.47
2:B:151:ALA:HB1	2:B:169:GLN:HG2	1.97	0.47
2:B:349[A]:HIS:HE1	2:B:511:LYS:HE2	1.79	0.47
1:C:565:LYS:HD3	1:C:566:GLU:OE2	2.15	0.47
2:D:396:VAL:CG2	2:D:651:LEU:HD21	2.45	0.47
1:A:619:ASP:O	1:A:620:LEU:C	2.52	0.47
1:C:570:ARG:HD3	1:C:570:ARG:HA	1.62	0.47
2:B:188:TYR:OH	2:B:206:LYS:HD3	2.15	0.47
2:B:189:SER:HB3	2:B:213:ASN:OD1	2.14	0.47
2:B:380:LYS:HD3	2:B:385:GLU:OE1	2.15	0.47
2:B:625:GLU:O	2:B:626:THR:OG1	2.29	0.47
2:B:308:ARG:O	2:B:308:ARG:HD2	2.15	0.46
1:C:594:GLN:CG	1:C:619:ASP:OD2	2.58	0.46
2:D:37:VAL:HG22	2:D:266:LEU:HD21	1.96	0.46
2:D:546:ASN:HA	2:D:547:PRO:HD3	1.74	0.46
1:A:436:GLU:O	1:A:485:SER:HB3	2.16	0.46
1:A:607:PHE:CZ	1:A:640:GLY:HA3	2.50	0.46
2:D:287:SER:OG	2:D:288:PRO:HD2	2.15	0.46
1:A:619:ASP:O	1:A:621:ASP:N	2.48	0.46
2:B:114:GLY:O	2:B:155:SER:HB3	2.14	0.46
1:C:393:LYS:HG2	1:C:394:ILE:N	2.31	0.46
1:C:446:GLU:CG	1:C:447:SER:H	2.27	0.46
2:D:218:ALA:HB2	2:D:221:ASP:OD2	2.15	0.46
2:D:536:GLN:O	2:D:539:PRO:HD2	2.15	0.46
1:A:265:ASN:ND2	2:B:527:LYS:HA	2.31	0.46
1:A:613:THR:CG2	1:A:633:ILE:HB	2.44	0.46
2:B:29:VAL:HG12	2:B:30:ILE:HD13	1.98	0.46
2:B:315:LEU:HD22	2:B:319:TYR:CE2	2.51	0.46
2:D:151:ALA:HB1	2:D:169:GLN:HG2	1.97	0.46
2:D:234:PRO:CD	2:D:237:GLU:HG3	2.36	0.46
2:B:453:ALA:HA	2:B:486:PRO:HD2	1.96	0.46
2:D:409:ALA:HB2	2:D:641:LEU:HD21	1.96	0.46
1:A:475:THR:O	1:A:476:LYS:HG2	2.16	0.46
2:B:344:TRP:HZ3	2:B:601:LEU:HD11	1.80	0.46
1:C:206:LYS:HE2	1:C:212:TYR:OH	2.16	0.46
1:C:345:LYS:CE	1:C:348:ASP:OD1	2.63	0.46
1:C:38:GLN:NE2	6:C:824:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:GLY:HA3	2:D:171:CYS:SG	2.56	0.46
1:A:588:ALA:HB3	1:A:594:GLN:CB	2.46	0.46
2:B:380:LYS:O	2:B:383:ASN:HB2	2.15	0.46
2:D:400:GLY:HA3	2:D:647:TYR:CG	2.51	0.46
2:D:75:ASN:N	2:D:75:ASN:OD1	2.48	0.46
1:A:610:THR:HA	1:A:636:ALA:O	2.16	0.46
1:A:594:GLN:CG	1:A:619:ASP:OD2	2.61	0.46
2:B:462:ILE:HB	2:B:463:PRO:CD	2.46	0.46
1:C:548:TRP:HB3	1:C:682:PHE:HB3	1.98	0.46
1:C:552:ILE:HD11	1:C:631:ALA:CB	2.46	0.46
2:D:11:VAL:CG1	2:D:11:VAL:O	2.64	0.46
2:D:309:MET:HE2	2:D:313:MET:HG2	1.97	0.46
2:D:625:GLU:O	2:D:626:THR:OG1	2.26	0.46
1:A:227:ASN:ND2	1:A:227:ASN:N	2.64	0.45
1:A:587:THR:HG21	1:A:592:GLN:HE22	1.77	0.45
2:B:89:GLU:OE1	2:B:89:GLU:N	2.49	0.45
1:C:129:HIS:CD2	1:C:129:HIS:N	2.84	0.45
1:A:134:TYR:O	1:A:167:GLY:HA2	2.16	0.45
1:A:552:ILE:HD11	1:A:631:ALA:CB	2.47	0.45
1:C:618:PHE:O	1:C:619:ASP:CB	2.65	0.45
2:D:188:TYR:OH	2:D:206:LYS:HD3	2.16	0.45
2:D:498:CYS:HB3	2:D:512:GLU:OE1	2.16	0.45
1:A:548:TRP:CD1	1:A:548:TRP:N	2.84	0.45
2:B:95:TYR:OH	3:B:703:GOL:H12	2.17	0.45
1:C:281:ASP:O	1:C:291:GLY:HA3	2.16	0.45
2:D:79:PRO:HB3	2:D:250:THR:HG21	1.97	0.45
1:A:585:LYS:HG3	1:A:585:LYS:O	2.15	0.45
1:C:73:LEU:HD12	1:C:74:PRO:CD	2.46	0.45
1:C:436:GLU:O	1:C:485:SER:HB3	2.17	0.45
2:D:214:LEU:HB2	2:D:220:ARG:CG	2.46	0.45
2:D:217:LYS:HG3	2:D:220:ARG:NH1	2.31	0.45
2:D:315:LEU:HD22	2:D:319:TYR:CE2	2.52	0.45
2:D:381:ILE:O	2:D:590:ARG:HD3	2.17	0.45
1:A:246:VAL:HG13	1:A:284:ILE:HD11	1.99	0.45
1:A:552:ILE:HD12	1:A:677:SER:O	2.17	0.45
2:D:188:TYR:CZ	2:D:206:LYS:HD3	2.52	0.45
1:A:46:ARG:HB2	1:A:162:TYR:CE1	2.52	0.45
1:A:129:HIS:CG	1:A:183:LYS:HB2	2.52	0.45
1:A:594:GLN:HB3	1:A:618:PHE:CE2	2.52	0.45
2:B:555:ASN:HB2	2:B:558:ASP:OD1	2.16	0.45
1:A:133:GLN:HB3	2:D:31:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349[A]:HIS:CE1	2:B:511:LYS:HE2	2.52	0.45
2:B:477:ASP:N	2:B:477:ASP:OD1	2.47	0.45
2:D:114:GLY:O	2:D:155:SER:HB3	2.17	0.45
2:D:354:LYS:HD3	2:D:630:LEU:HD12	1.98	0.45
1:A:186:TRP:CE2	1:A:257:LEU:HB3	2.51	0.45
1:A:244:LEU:N	1:A:244:LEU:HD12	2.31	0.45
2:B:228:LEU:HA	2:B:228:LEU:HD23	1.77	0.45
1:C:552:ILE:HD12	1:C:677:SER:O	2.17	0.45
2:D:308:ARG:HD2	2:D:308:ARG:O	2.17	0.45
2:D:90:ASP:N	2:D:91:PRO:HD3	2.32	0.45
1:A:206:LYS:NZ	6:B:801:HOH:O	2.47	0.44
2:D:29:VAL:HG12	2:D:30:ILE:HD13	1.99	0.44
2:D:335:PRO:HA	2:D:336:THR:HA	1.43	0.44
2:D:554:LEU:HA	2:D:554:LEU:HD23	1.79	0.44
2:B:524:LEU:HB2	2:B:531:ALA:HB2	1.99	0.44
2:B:188:TYR:OH	3:B:704:GOL:H2	2.18	0.44
1:C:613:THR:CG2	1:C:633:ILE:HB	2.47	0.44
6:C:834:HOH:O	2:D:353:LEU:CD1	2.65	0.44
1:A:155:ILE:HD12	2:B:360:VAL:HG21	2.00	0.44
1:A:617:GLY:HA2	1:A:631:ALA:O	2.16	0.44
1:C:327:LEU:HD12	1:C:327:LEU:C	2.38	0.44
2:D:555:ASN:HB2	2:D:558:ASP:OD1	2.17	0.44
1:A:615:GLU:HA	1:A:616:SER:HA	1.60	0.44
1:A:606:GLY:HA2	1:A:641:GLY:HA2	2.00	0.44
2:B:85:TYR:N	2:B:85:TYR:CD2	2.86	0.44
1:C:80:LEU:HD13	1:C:140:PHE:CG	2.53	0.44
1:C:619:ASP:O	1:C:627:ARG:O	2.35	0.44
2:D:218:ALA:HA	2:D:221:ASP:CG	2.38	0.44
2:D:340:LYS:HB3	2:D:341:PRO:HD2	1.99	0.44
2:D:396:VAL:HG22	2:D:651:LEU:HD21	1.98	0.44
1:A:565:LYS:HB2	1:A:566:GLU:CA	2.46	0.44
2:B:505:LEU:O	2:B:506:CYS:HB3	2.18	0.44
1:C:554:ASN:HB2	1:C:676:SER:HG	1.80	0.44
1:C:585:LYS:HG3	1:C:585:LYS:O	2.18	0.44
2:B:400:GLY:HA3	2:B:647:TYR:CG	2.53	0.43
1:C:481:GLU:O	1:C:493:GLY:HA3	2.18	0.43
1:C:531:THR:HB	1:C:644:GLY:O	2.18	0.43
2:D:289:HIS:CD2	2:D:289:HIS:N	2.86	0.43
1:A:383:ASP:O	1:A:527:GLN:HA	2.18	0.43
2:B:306:PRO:HA	2:B:307:PRO:HD3	1.88	0.43
1:C:617:GLY:HA2	1:C:631:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:HIS:CD2	2:D:289:HIS:H	2.36	0.43
1:A:535:GLU:OE2	1:A:645:PRO:HA	2.19	0.43
2:B:381:ILE:O	2:B:590:ARG:HD3	2.18	0.43
1:A:565:LYS:HD3	1:A:566:GLU:OE2	2.18	0.43
1:C:386:GLU:C	1:C:387:LEU:HD12	2.39	0.43
1:C:548:TRP:N	1:C:548:TRP:CD1	2.86	0.43
1:A:585:LYS:HA	1:A:596:PHE:O	2.18	0.43
1:A:481:GLU:O	1:A:493:GLY:HA3	2.19	0.43
1:C:288:ARG:HD3	3:C:701:GOL:C3	2.32	0.43
2:D:80:VAL:O	2:D:305:VAL:HB	2.19	0.43
2:B:625:GLU:OE1	2:B:625:GLU:HA	2.19	0.43
1:C:288:ARG:HH21	1:C:402:ASN:HB2	1.82	0.43
2:D:534:LYS:HD2	2:D:632:ARG:NH2	2.34	0.43
1:A:214:GLY:HA2	6:A:804:HOH:O	2.19	0.43
2:B:180:SER:OG	2:B:182:LEU:HB2	2.19	0.43
2:B:311:ALA:O	2:B:315:LEU:HD12	2.19	0.43
1:C:70:ALA:O	1:C:83:ARG:NH1	2.52	0.43
2:D:400:GLY:HA3	2:D:647:TYR:CD1	2.53	0.43
2:D:625:GLU:OE1	2:D:625:GLU:HA	2.19	0.43
1:A:73:LEU:HD12	1:A:74:PRO:HD2	2.00	0.42
2:B:107:PHE:HA	2:B:111:GLN:OE1	2.19	0.42
2:B:262:LEU:HA	2:B:262:LEU:HD12	1.71	0.42
2:B:546:ASN:HA	2:B:547:PRO:HD3	1.76	0.42
2:B:663:ARG:NH1	6:B:855:HOH:O	2.52	0.42
1:C:610:THR:HA	1:C:636:ALA:O	2.19	0.42
2:B:340:LYS:HB3	2:B:341:PRO:HD2	2.01	0.42
2:B:392:ASP:N	6:B:864:HOH:O	2.48	0.42
1:C:188:PHE:CE2	1:C:216:SER:HB3	2.54	0.42
1:C:214:GLY:HA2	6:C:807:HOH:O	2.19	0.42
1:C:253:LEU:HD12	1:C:253:LEU:C	2.39	0.42
1:C:591:ARG:HA	1:C:592:GLN:HA	1.70	0.42
2:D:490:LYS:HE3	2:D:503:LEU:O	2.19	0.42
2:B:520:ALA:O	2:B:523:CYS:HB3	2.20	0.42
1:C:436:GLU:HG3	1:C:437:PHE:N	2.34	0.42
1:A:309:VAL:HG12	1:A:310:SER:N	2.34	0.42
1:A:418:LYS:O	1:A:419:ASP:C	2.57	0.42
1:A:570:ARG:HA	1:A:570:ARG:HD3	1.65	0.42
1:C:535:GLU:OE2	1:C:645:PRO:HA	2.19	0.42
2:D:642:HIS:HB3	2:D:643:ASP:OD1	2.20	0.42
1:A:124:ASN:HD22	1:A:185:VAL:HG11	1.84	0.42
1:A:386:GLU:C	1:A:387:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:VAL:HB	2:B:225:LEU:HD22	2.01	0.42
2:B:554:LEU:HD22	2:B:559:TYR:OH	2.20	0.42
1:A:124:ASN:HD21	1:A:185:VAL:HB	1.84	0.42
2:B:462:ILE:N	2:B:463:PRO:HD2	2.35	0.42
2:B:642:HIS:HB3	2:B:643:ASP:OD1	2.20	0.42
2:B:646:THR:CG2	2:B:649:LYS:HD2	2.41	0.42
1:C:134:TYR:O	1:C:167:GLY:HA2	2.20	0.42
1:C:330:ARG:HA	1:C:340:VAL:O	2.20	0.42
2:D:107:PHE:HA	2:D:111:GLN:OE1	2.19	0.42
2:D:80:VAL:CG1	2:D:260:GLU:HG2	2.49	0.42
2:D:563:CYS:N	2:D:577:CYS:SG	2.93	0.42
1:A:50:ARG:HD2	1:A:58:GLU:O	2.20	0.41
2:B:489:LYS:HD2	2:B:489:LYS:HA	1.94	0.41
2:D:539:PRO:O	2:D:545:LYS:HD2	2.19	0.41
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.71	0.41
1:C:526:LEU:HD22	1:C:653:TRP:CE3	2.55	0.41
1:A:591:ARG:HA	1:A:592:GLN:HA	1.78	0.41
2:B:546:ASN:C	2:B:546:ASN:OD1	2.58	0.41
1:C:573:PHE:CZ	1:C:682:PHE:CE1	3.08	0.41
1:A:206:LYS:NZ	6:A:833:HOH:O	2.53	0.41
2:B:539:PRO:O	2:B:545:LYS:HD2	2.20	0.41
1:C:244:LEU:HD23	1:C:253:LEU:HD13	2.01	0.41
2:B:309:MET:HG2	2:B:314:TYR:HB2	2.02	0.41
2:B:500:GLY:HA3	2:B:505:LEU:HA	2.02	0.41
1:C:329:PHE:CZ	1:C:342:GLY:HA3	2.55	0.41
1:C:400:PHE:O	1:C:401:SER:HB2	2.20	0.41
2:D:89:GLU:N	2:D:89:GLU:OE1	2.53	0.41
2:D:95:TYR:CE2	2:D:246:VAL:HG22	2.56	0.41
1:A:418:LYS:N	1:A:418:LYS:HD3	2.34	0.41
1:A:483:CYS:HA	1:A:484:CYS:HA	1.89	0.41
1:A:489:TYR:CE2	1:A:645:PRO:HD2	2.55	0.41
2:B:146:LEU:HA	2:B:146:LEU:HD12	1.89	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.82	0.41
1:C:184:GLY:HA3	1:C:343:SER:O	2.21	0.41
1:C:288:ARG:NH2	1:C:402:ASN:HB2	2.36	0.41
1:C:383:ASP:O	1:C:527:GLN:HA	2.21	0.41
1:C:615:GLU:HA	1:C:616:SER:HA	1.59	0.41
2:B:392:ASP:O	2:B:395:PHE:N	2.54	0.41
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.90	0.41
1:A:400:PHE:O	1:A:401:SER:HB2	2.20	0.41
1:C:223:TYR:OH	2:D:549:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:TYR:CD2	2:D:85:TYR:N	2.88	0.41
1:A:582:ILE:HG23	1:A:582:ILE:O	2.20	0.41
1:A:270:ASN:C	1:A:272:LYS:H	2.24	0.41
2:D:473:HIS:HE1	2:D:475:ARG:O	2.03	0.41
2:D:524:LEU:HB2	2:D:531:ALA:HB2	2.02	0.41
1:A:171:SER:OG	1:A:324:GLY:HA2	2.21	0.41
1:A:556:THR:HG22	1:A:620:LEU:CG	2.38	0.41
1:A:619:ASP:OD1	1:A:621:ASP:CB	2.69	0.41
2:D:119:HIS:N	2:D:119:HIS:CD2	2.89	0.41
2:D:494:LEU:HD23	2:D:494:LEU:HA	1.83	0.41
1:A:147:GLU:O	1:A:155:ILE:HA	2.21	0.40
1:A:150:PHE:HE2	1:A:155:ILE:HD13	1.86	0.40
1:A:49:ARG:HG2	1:A:157:SER:O	2.21	0.40
1:A:304:LYS:HD3	1:A:304:LYS:HA	1.74	0.40
2:B:638:LEU:HA	2:B:638:LEU:HD23	1.90	0.40
2:B:228:LEU:HB2	3:B:706:GOL:H2	2.02	0.40
2:D:113:ARG:NH2	2:D:138:ASP:O	2.54	0.40
2:D:349[A]:HIS:ND1	6:D:849:HOH:O	2.54	0.40
2:D:601:LEU:HD23	2:D:601:LEU:HA	1.61	0.40
2:D:125:SER:N	3:D:703:GOL:H2	2.36	0.40
2:B:185:TYR:HE1	2:B:193:LYS:HG2	1.86	0.40
2:B:90:ASP:N	2:B:91:PRO:HD3	2.36	0.40
1:C:163:ILE:HD12	1:C:341:VAL:HG22	2.02	0.40
1:C:270:ASN:OD1	1:C:271:ASP:N	2.45	0.40
1:C:408:VAL:O	1:C:411:ILE:HG13	2.20	0.40
2:D:210[A]:ILE:HD13	2:D:235:VAL:HG21	2.02	0.40
2:D:392:ASP:O	2:D:395:PHE:N	2.53	0.40
1:A:206:LYS:HE2	1:A:212:TYR:OH	2.20	0.40
2:B:192:PHE:CE1	2:B:210:ILE:HD12	2.56	0.40
2:B:400:GLY:HA3	2:B:647:TYR:CD1	2.57	0.40
2:D:210[A]:ILE:HD13	2:D:235:VAL:CG1	2.43	0.40
2:D:311:ALA:O	2:D:315:LEU:HD12	2.21	0.40
1:A:50:ARG:NH2	1:A:210:ASP:OD1	2.39	0.40
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.76	0.40
2:B:349[B]:HIS:NE2	2:B:353:LEU:CD1	2.84	0.40
2:B:381:ILE:HD13	2:B:388:ALA:HA	2.03	0.40
1:C:147:GLU:O	1:C:155:ILE:HA	2.21	0.40
2:D:443:ASN:CG	2:D:443:ASN:O	2.60	0.40
1:A:475:THR:O	1:A:476:LYS:CG	2.69	0.40
1:A:80:LEU:HD13	1:A:140:PHE:CG	2.57	0.40
1:C:150:PHE:HE2	1:C:155:ILE:HD13	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:MET:HG2	2:D:314:TYR:HB2	2.04	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	522/658 (79%)	501 (96%)	20 (4%)	1 (0%)	51	84
1	C	518/658 (79%)	497 (96%)	21 (4%)	0	100	100
2	B	673/679 (99%)	639 (95%)	34 (5%)	0	100	100
2	D	678/679 (100%)	650 (96%)	28 (4%)	0	100	100
All	All	2391/2674 (89%)	2287 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	LYS

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	455/533 (85%)	417 (92%)	38 (8%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	452/533 (85%)	411 (91%)	41 (9%)	11	36
2	B	571/572 (100%)	536 (94%)	35 (6%)	22	56
2	D	573/572 (100%)	538 (94%)	35 (6%)	22	56
All	All	2051/2210 (93%)	1902 (93%)	149 (7%)	16	48

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	94	ASP
1	A	97	SER
1	A	123	LYS
1	A	124	ASN
1	A	148	LYS
1	A	155	ILE
1	A	166	HIS
1	A	172	ARG
1	A	220	SER
1	A	222	GLU
1	A	227	ASN
1	A	253	LEU
1	A	264	LEU
1	A	267	ASN
1	A	303	THR
1	A	316	SER
1	A	337	LYS
1	A	338	VAL
1	A	345	LYS
1	A	391	ASP
1	A	401	SER
1	A	444	THR
1	A	531	THR
1	A	552	ILE
1	A	556	THR
1	A	557	SER
1	A	566	GLU
1	A	570	ARG
1	A	574	THR
1	A	579	ASP
1	A	592	GLN
1	A	596	PHE

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Mol	Chain	Res	Type
1	A	597	THR
1	A	619	ASP
1	A	635	ASP
1	A	660	LYS
1	A	676	SER
2	B	17	THR
2	B	33	ASP
2	B	40	VAL
2	B	46	LEU
2	B	71	TYR
2	B	102	LYS
2	B	124	ARG
2	B	125	SER
2	B	141	GLU
2	B	216	ASN
2	B	235	VAL
2	B	246	VAL
2	B	249	HIS
2	B	251	VAL
2	B	260	GLU
2	B	261	ASP
2	B	309	MET
2	B	330	THR
2	B	347	LEU
2	B	353	LEU
2	B	370	SER
2	B	377	CYS
2	B	396	VAL
2	B	413	ASP
2	B	438	ASP
2	B	439	LEU
2	B	440	THR
2	B	475	ARG
2	B	505	LEU
2	B	572	GLU
2	B	589	THR
2	B	591	LYS
2	B	625	GLU
2	B	643	ASP
2	B	646	THR
1	C	66	SER
1	C	94	ASP

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Mol	Chain	Res	Type
1	C	97	SER
1	C	120	ASN
1	C	123	LYS
1	C	124	ASN
1	C	148	LYS
1	C	155	ILE
1	C	166	HIS
1	C	172	ARG
1	C	220	SER
1	C	222	GLU
1	C	227	ASN
1	C	253	LEU
1	C	264	LEU
1	C	267	ASN
1	C	302	GLU
1	C	303	THR
1	C	316	SER
1	C	337	LYS
1	C	338	VAL
1	C	345	LYS
1	C	375	ASN
1	C	391	ASP
1	C	419	ASP
1	C	444	THR
1	C	531	THR
1	C	552	ILE
1	C	556	THR
1	C	557	SER
1	C	566	GLU
1	C	570	ARG
1	C	574	THR
1	C	579	ASP
1	C	592	GLN
1	C	596	PHE
1	C	597	THR
1	C	619	ASP
1	C	627	ARG
1	C	635	ASP
1	C	676	SER
2	D	17	THR
2	D	33	ASP
2	D	40	VAL

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Mol	Chain	Res	Type
2	D	46	LEU
2	D	71	TYR
2	D	75	ASN
2	D	102	LYS
2	D	124	ARG
2	D	125	SER
2	D	141	GLU
2	D	219	ASP
2	D	246	VAL
2	D	249	HIS
2	D	251	VAL
2	D	260	GLU
2	D	309	MET
2	D	330	THR
2	D	336	THR
2	D	347	LEU
2	D	353	LEU
2	D	370	SER
2	D	377	CYS
2	D	396	VAL
2	D	413	ASP
2	D	438	ASP
2	D	439	LEU
2	D	440	THR
2	D	475	ARG
2	D	505	LEU
2	D	572	GLU
2	D	589	THR
2	D	591	LYS
2	D	625	GLU
2	D	643	ASP
2	D	646	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	227	ASN
1	A	265	ASN
1	A	592	GLN
2	B	75	ASN
2	B	289	HIS

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Mol	Chain	Res	Type
1	C	124	ASN
1	C	227	ASN
1	C	592	GLN
2	D	289	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	GOL	A	701	-	5,5,5	0.35	0	5,5,5	0.24	0
3	GOL	A	702	-	5,5,5	0.31	0	5,5,5	0.58	0
4	CO3	B	701	5	0,3,3	0.00	-	0,3,3	0.00	-
3	GOL	B	703	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	B	704	-	5,5,5	0.52	0	5,5,5	0.72	0
3	GOL	B	705	-	5,5,5	0.28	0	5,5,5	0.60	0
3	GOL	B	706	-	5,5,5	0.48	0	5,5,5	0.71	0
3	GOL	B	707	-	5,5,5	0.37	0	5,5,5	0.78	0
3	GOL	B	708	-	5,5,5	0.32	0	5,5,5	0.47	0
3	GOL	C	701	-	5,5,5	0.38	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CO3	D	701	5	0,3,3	0.00	-	0,3,3	0.00	-
3	GOL	D	703	-	5,5,5	0.38	0	5,5,5	0.54	0
3	GOL	D	704	-	5,5,5	0.31	0	5,5,5	0.43	0
3	GOL	D	705	-	5,5,5	0.22	0	5,5,5	0.71	0
3	GOL	D	706	-	5,5,5	0.46	0	5,5,5	0.65	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	GOL	A	701	-	-	0/4/4/4	0/0/0/0
3	GOL	A	702	-	-	0/4/4/4	0/0/0/0
4	CO3	B	701	5	-	0/0/0/0	0/0/0/0
3	GOL	B	703	-	-	0/4/4/4	0/0/0/0
3	GOL	B	704	-	-	0/4/4/4	0/0/0/0
3	GOL	B	705	-	-	0/4/4/4	0/0/0/0
3	GOL	B	706	-	-	0/4/4/4	0/0/0/0
3	GOL	B	707	-	-	0/4/4/4	0/0/0/0
3	GOL	B	708	-	-	0/4/4/4	0/0/0/0
3	GOL	C	701	-	-	0/4/4/4	0/0/0/0
4	CO3	D	701	5	-	0/0/0/0	0/0/0/0
3	GOL	D	703	-	-	0/4/4/4	0/0/0/0
3	GOL	D	704	-	-	0/4/4/4	0/0/0/0
3	GOL	D	705	-	-	0/4/4/4	0/0/0/0
3	GOL	D	706	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	GOL	2	0
3	B	703	GOL	1	0
3	B	704	GOL	5	0
3	B	706	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	707	GOL	1	0
3	C	701	GOL	3	0
3	D	703	GOL	4	0
3	D	705	GOL	1	0

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

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, 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	537/658 (81%)	0.43	60 (11%) 6 3	35, 67, 136, 216	13 (2%)
1	C	536/658 (81%)	0.36	49 (9%) 10 5	37, 65, 143, 191	6 (1%)
2	B	675/679 (99%)	0.15	16 (2%) 59 40	30, 60, 105, 205	7 (1%)
2	D	677/679 (99%)	0.15	21 (3%) 49 31	30, 58, 101, 179	9 (1%)
All	All	2425/2674 (90%)	0.26	146 (6%) 23 13	30, 62, 124, 216	35 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	VAL	9.4
1	C	616	SER	8.2
1	A	632	TYR	6.6
1	A	268	THR	6.4
1	C	119	VAL	6.2
1	C	593	ALA	6.1
1	A	303	THR	6.1
1	A	299	LYS	5.8
1	A	620	LEU	5.8
2	B	417[A]	ASN	5.8
1	C	554	ASN	5.7
1	C	630	LYS	5.4
2	D	335	PRO	5.3
1	C	632	TYR	5.3
1	A	631	ALA	5.3
1	A	266	ASN	5.1
2	D	89	GLU	4.9
1	A	616	SER	4.8
1	A	120	ASN	4.8
1	C	590	ASN	4.6
1	A	150	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	617	GLY	4.5
1	C	420	SER	4.5
1	A	301	ASN	4.3
1	C	635	ASP	4.2
2	B	87	SER	4.2
2	B	333	GLU	4.2
1	A	633	ILE	4.2
1	A	618	PHE	4.2
2	B	438	ASP	4.1
1	C	629	PRO	4.1
1	C	675	ALA	4.1
1	C	691	GLN	4.1
1	A	630	LYS	4.0
2	B	420	ASP	3.8
1	C	120	ASN	3.8
1	A	635	ASP	3.7
1	C	350	LEU	3.7
1	C	419	ASP	3.6
1	C	118	GLY	3.6
2	D	333	GLU	3.6
1	A	441	PHE	3.5
1	A	475	THR	3.5
1	C	631	ALA	3.4
2	D	88	LYS	3.4
1	A	629	PRO	3.4
2	D	417	ASN	3.4
1	C	520	VAL	3.3
2	B	86	GLY	3.3
1	C	108	SER	3.3
1	C	676	SER	3.3
1	A	265	ASN	3.3
1	A	519	GLN	3.3
2	B	472	ASN	3.3
1	A	269	ASN	3.2
2	D	482	GLU	3.2
1	A	634	THR	3.2
2	D	336	THR	3.2
2	D	496	LYS	3.2
2	B	88	LYS	3.1
1	A	350	LEU	3.1
1	A	499	ASN	3.1
1	C	375	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	498	LYS	3.1
1	A	271	ASP	3.1
1	C	267	ASN	2.9
1	A	442	GLU	2.9
1	C	634	THR	2.9
1	A	564	ASP	2.9
1	A	376	SER	2.9
1	C	628	THR	2.9
1	A	688	GLN	2.9
2	D	481	SER	2.9
1	C	374	GLU	2.9
1	A	53	TYR	2.8
1	C	565	LYS	2.8
1	A	444	THR	2.7
1	C	440	LYS	2.7
1	C	442	GLU	2.7
1	C	556	THR	2.6
2	D	435	SER	2.6
1	A	621	ASP	2.6
1	A	267	ASN	2.6
1	C	499	ASN	2.6
1	C	566	GLU	2.6
1	C	555	GLY	2.6
1	A	477	THR	2.6
1	C	300	GLU	2.5
1	A	659	ASP	2.5
2	B	615	CYS	2.5
2	D	438	ASP	2.5
2	D	436	ALA	2.5
2	D	470	LYS	2.5
2	D	90	ASP	2.4
2	B	642	HIS	2.4
1	A	689	PRO	2.4
1	A	596	PHE	2.4
1	A	108	SER	2.4
1	C	552	ILE	2.4
1	C	303	THR	2.4
1	A	676	SER	2.4
1	A	109	ASN	2.4
1	C	498	LYS	2.4
2	B	192	PHE	2.4
1	C	687	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	478	TYR	2.3
1	C	349	LYS	2.3
1	C	615	GLU	2.3
1	C	417	PRO	2.3
1	C	418	LYS	2.3
1	A	480	VAL	2.3
2	B	643	ASP	2.3
1	A	617	GLY	2.3
1	A	154	LYS	2.2
1	C	444	THR	2.2
1	C	567	GLY	2.2
1	A	565	LYS	2.2
2	D	332	PRO	2.2
2	B	479	PHE	2.2
1	C	592	GLN	2.2
1	A	151	SER	2.1
1	A	446	GLU	2.1
1	A	309	VAL	2.1
2	D	337	ASP	2.1
1	A	479	GLU	2.1
1	A	615	GLU	2.1
2	B	155	SER	2.1
1	A	619	ASP	2.1
1	C	636	ALA	2.1
2	D	416	ASP	2.1
2	D	658	ALA	2.1
1	A	557	SER	2.1
1	A	482	VAL	2.1
2	B	349[A]	HIS	2.1
1	C	264	LEU	2.1
2	D	467	LEU	2.1
1	A	419	ASP	2.1
2	B	421	THR	2.1
2	D	86	GLY	2.1
2	D	612	VAL	2.1
1	C	614	ALA	2.0
1	A	110	HIS	2.0
1	A	443	HIS	2.0
1	C	149	ASP	2.0
1	A	592	GLN	2.0
1	A	56	ALA	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	707	6/6	0.90	0.32	5.41	57,57,57,57	0
3	GOL	B	703	6/6	0.87	0.30	5.36	48,48,48,48	6
3	GOL	C	701	6/6	0.96	0.30	3.81	60,60,60,60	0
3	GOL	B	708	6/6	0.74	0.36	2.42	127,127,127,127	0
3	GOL	B	705	6/6	0.86	0.24	2.00	76,76,76,76	0
3	GOL	D	705	6/6	0.90	0.24	1.71	43,43,43,43	6
3	GOL	A	702	6/6	0.89	0.24	1.49	38,38,38,38	6
3	GOL	B	706	6/6	0.89	0.22	0.60	53,53,53,53	0
3	GOL	D	706	6/6	0.94	0.17	0.38	44,44,44,44	6
3	GOL	B	704	6/6	0.91	0.21	0.11	52,52,52,52	0
3	GOL	A	701	6/6	0.88	0.29	-0.17	50,50,50,50	6
3	GOL	D	704	6/6	0.95	0.17	-0.30	65,65,65,65	0
3	GOL	D	703	6/6	0.93	0.19	-0.44	51,51,51,51	0
4	CO3	D	701	4/4	0.99	0.17	-0.75	48,48,48,48	0
5	FE	D	702	1/1	1.00	0.16	-0.84	44,44,44,44	0
4	CO3	B	701	4/4	0.99	0.13	-1.33	36,36,36,36	0
5	FE	B	702	1/1	0.98	0.14	-1.57	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.