Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 – 11:38 PM BST

PDB ID	:	6CSE
Title	:	Crystal structure of sodium/alanine symporter AgcS with L-alanine bound
Authors	:	Ma, J.; Reyes, F.E.; Gonen, T.
Deposited on	:	2018-03-20
Resolution	:	3.24 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 (i) symbol.

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

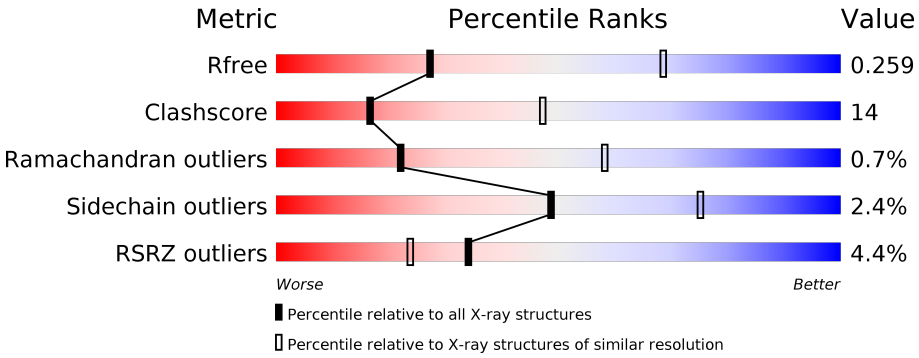
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 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	214	3% 80% 19%
1	H	214	% 83% 16%
2	B	213	% 79% 21%
2	L	213	% 77% 23%
3	C	453	8% 62% 30% 6%
3	M	453	6% 61% 33% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ALA	M	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12670 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 Monoclonal antibody FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1556	973	259	315	9			
1	H	214	Total	C	N	O	S	0	0	0
			1556	973	259	315	9			

- Molecule 2 is a protein called Monoclonal antibody FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1606	998	273	328	7			
2	L	213	Total	C	N	O	S	0	0	0
			1606	998	273	328	7			

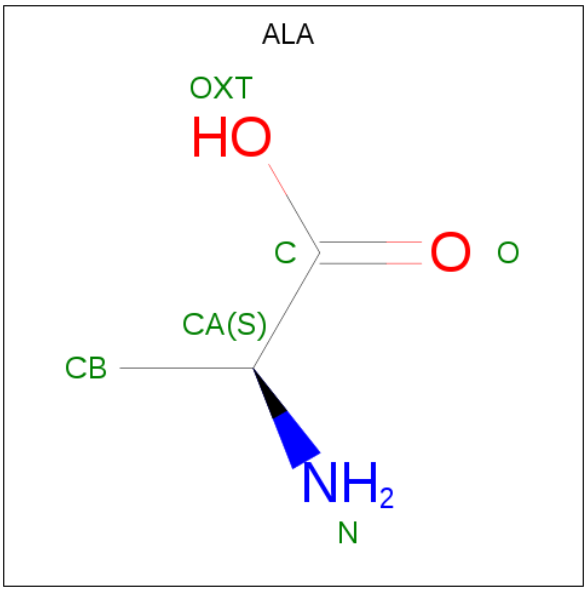
- Molecule 3 is a protein called Sodium/alanine symporter AgcS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	431	Total	C	N	O	S	0	0	0
			3183	2113	498	555	17			
3	C	428	Total	C	N	O	S	0	0	0
			3156	2094	495	550	17			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Na	0	0
			1	1		

- Molecule 5 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



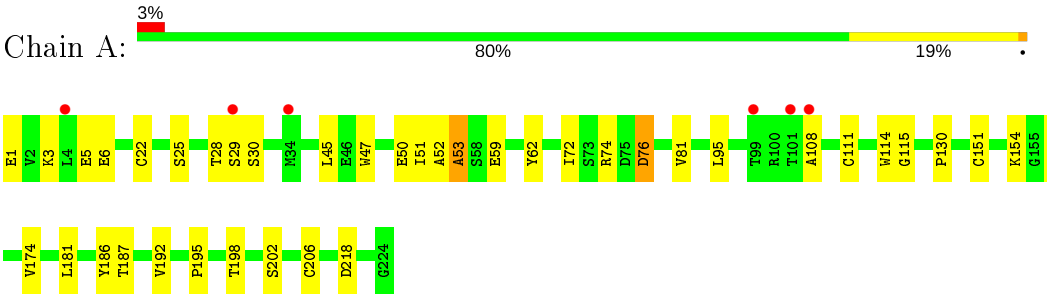
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	6	3	1	2	0	0

3 Residue-property plots

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

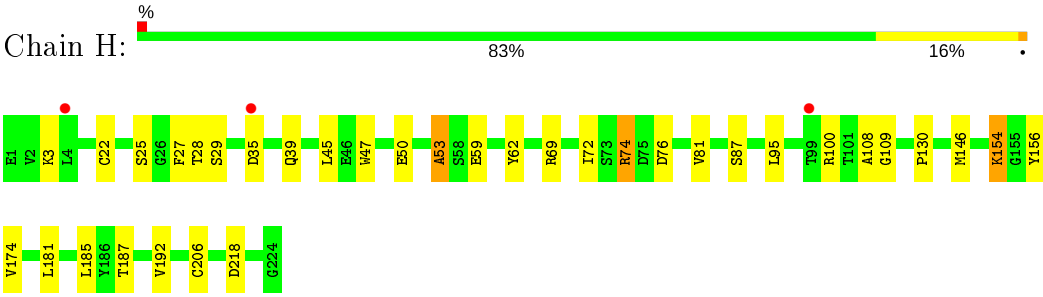
- Molecule 1: Monoclonal antibody FAB heavy chain

Chain A:



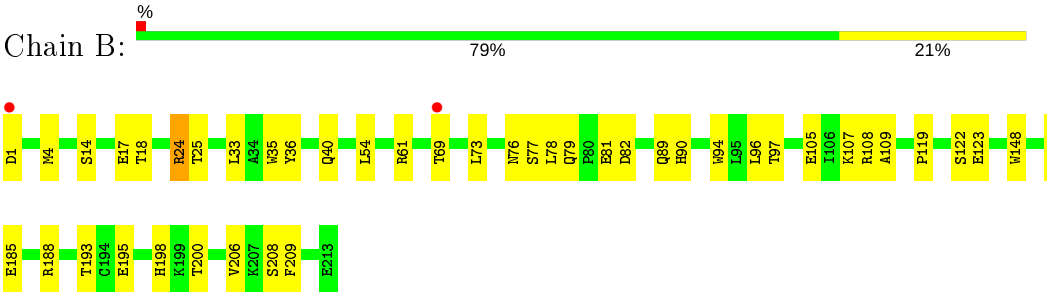
- Molecule 1: Monoclonal antibody FAB heavy chain

Chain H:



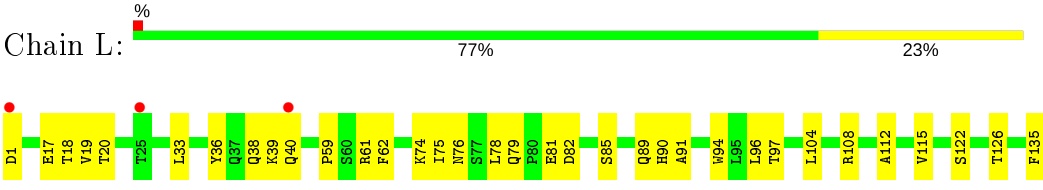
- Molecule 2: Monoclonal antibody FAB light chain

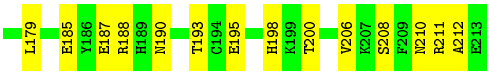
Chain B:



- Molecule 2: Monoclonal antibody FAB light chain

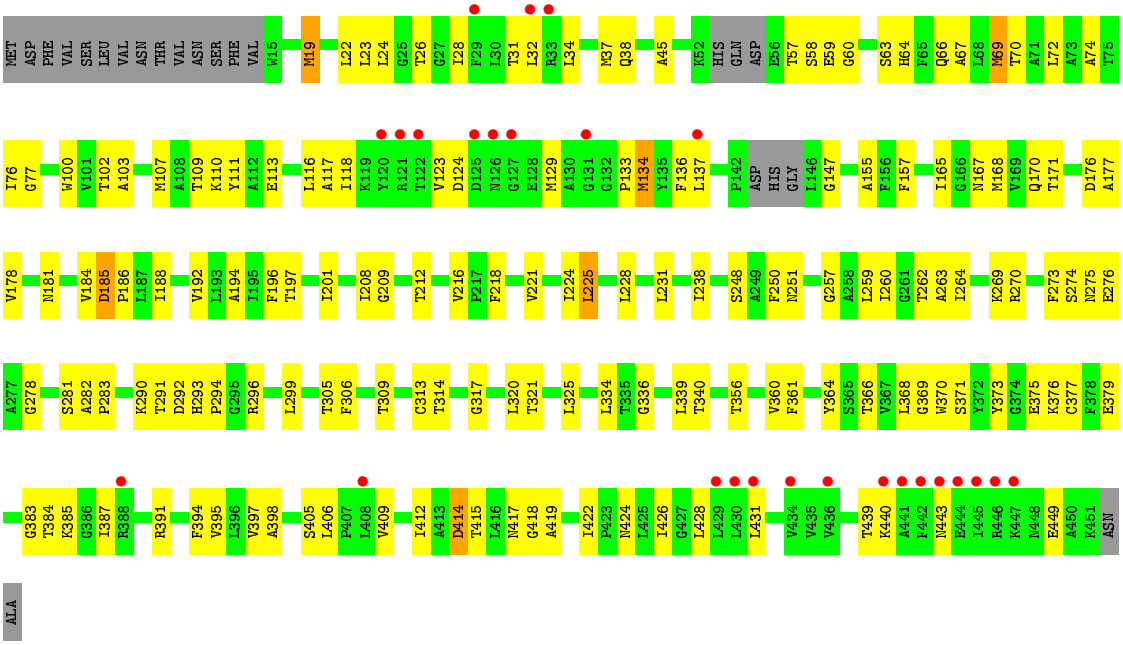
Chain L:





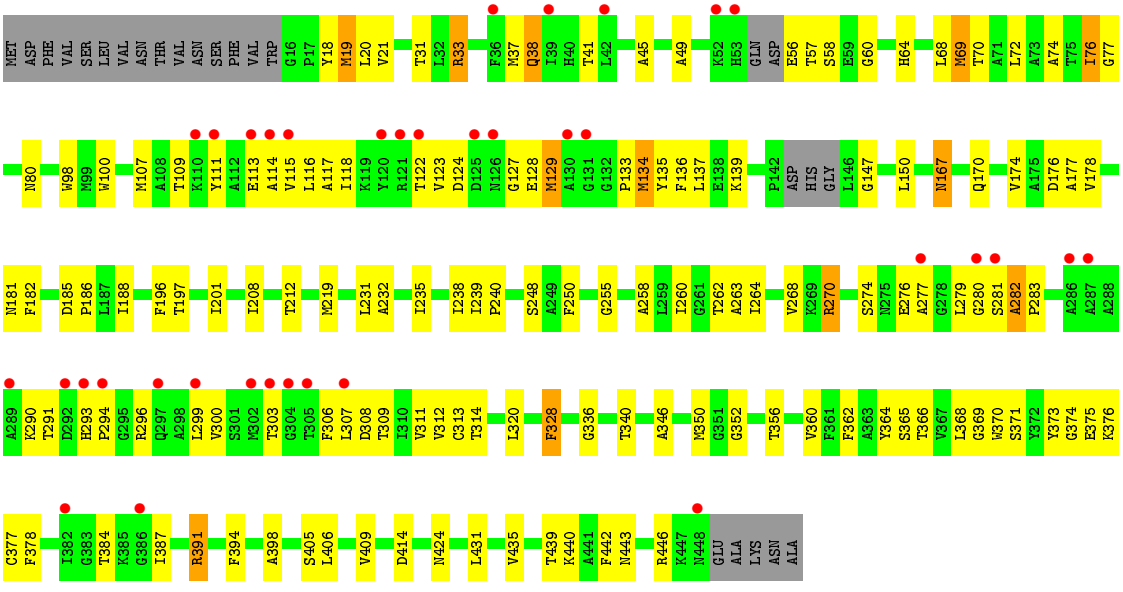
- Molecule 3: Sodium/alanine symporter AgcS

Chain M:



- Molecule 3: Sodium/alanine symporter AgcS

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	183.48Å 183.48Å 349.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.99 – 3.24 117.50 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.99-3.24) 99.9 (117.50-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.230 , 0.251 0.238 , 0.259	Depositor DCC
R_{free} test set	5187 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	105.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: NA

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	0.35	0/1593	0.55	0/2177
1	H	0.36	0/1593	0.55	0/2177
2	B	0.35	0/1639	0.56	0/2225
2	L	0.32	0/1639	0.55	0/2225
3	C	0.33	0/3229	0.47	0/4390
3	M	0.31	0/3257	0.47	0/4428
All	All	0.33	0/12950	0.51	0/17622

There are no bond length outliers.

There are no bond angle outliers.

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	1556	0	1510	28	0
1	H	1556	0	1510	24	0
2	B	1606	0	1554	38	0
2	L	1606	0	1554	33	0
3	C	3156	0	3246	127	0
3	M	3183	0	3272	123	0
4	M	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	6	0	4	7	0
All	All	12670	0	12650	359	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 (359) 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)
3:C:113:GLU:OE1	3:C:280:GLY:HA2	1.43	1.16
3:C:276:GLU:OE2	3:C:370:TRP:HZ2	1.45	1.00
3:C:49:ALA:HB2	3:C:300:VAL:HG22	1.46	0.95
3:C:276:GLU:OE2	3:C:370:TRP:CZ2	2.22	0.92
3:M:276:GLU:OE1	3:M:370:TRP:HZ2	1.53	0.91
3:C:387:ILE:O	3:C:391:ARG:HG2	1.71	0.90
3:M:276:GLU:OE1	3:M:370:TRP:CZ2	2.27	0.87
3:C:113:GLU:OE1	3:C:280:GLY:CA	2.25	0.85
3:C:281:SER:O	3:C:373:TYR:CE2	2.31	0.83
1:H:22:CYS:HB3	1:H:81:VAL:HG12	1.61	0.83
3:M:64:HIS:HE1	3:M:296:ARG:HG2	1.47	0.80
3:C:118:ILE:HG12	3:C:294:PRO:HD3	1.64	0.78
3:C:282:ALA:H	3:C:283:PRO:HD2	1.51	0.75
3:C:49:ALA:CB	3:C:300:VAL:HG22	2.17	0.75
1:H:130:PRO:HB3	1:H:156:TYR:HB3	1.69	0.75
1:A:174:VAL:HG12	1:A:192:VAL:HG23	1.68	0.74
3:C:113:GLU:HB3	3:C:283:PRO:HG3	1.68	0.74
3:C:177:ALA:O	3:C:181:ASN:ND2	2.21	0.74
3:C:100:TRP:HE1	3:C:314:THR:HG1	1.33	0.74
3:M:292:ASP:OD2	3:M:296:ARG:NH1	2.21	0.74
2:B:81:GLU:HG2	2:L:81:GLU:HG3	1.70	0.74
2:B:61:ARG:NH1	2:L:79:GLN:OE1	2.21	0.74
3:C:137:LEU:HD13	3:C:150:LEU:HB3	1.71	0.73
3:C:276:GLU:HG2	3:C:279:LEU:HD12	1.68	0.73
3:C:270:ARG:HE	3:C:270:ARG:HA	1.54	0.72
3:C:387:ILE:HG12	3:C:391:ARG:HE	1.55	0.71
3:C:167:ASN:HD21	3:C:398:ALA:HA	1.54	0.70
3:M:100:TRP:HE1	3:M:314:THR:HG1	1.34	0.70
3:M:406:LEU:HB3	3:M:409:VAL:HB	1.73	0.70
3:M:74:ALA:HA	3:M:366:THR:HA	1.72	0.70
3:M:276:GLU:CD	3:M:370:TRP:HZ2	1.94	0.70
3:C:201:ILE:O	3:C:391:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:270:ARG:NH2	3:C:414:ASP:OD2	2.25	0.70
3:C:100:TRP:NE1	3:C:314:THR:OG1	2.22	0.69
1:A:22:CYS:HB3	1:A:81:VAL:HG12	1.73	0.69
3:C:375:GLU:OE2	3:C:391:ARG:HD3	1.93	0.69
1:A:59:GLU:HB2	3:C:405:SER:HA	1.74	0.68
3:C:127:GLY:O	3:C:129:MET:N	2.22	0.68
3:M:113:GLU:HB3	3:M:283:PRO:HG3	1.74	0.68
3:C:80:ASN:ND2	3:C:308:ASP:OD2	2.24	0.68
3:C:18:TYR:O	3:C:21:VAL:HG22	1.94	0.68
3:M:405:SER:HA	1:H:59:GLU:HB2	1.75	0.68
1:H:29:SER:O	1:H:74:ARG:NH1	2.24	0.67
3:M:270:ARG:NH2	3:M:414:ASP:OD2	2.26	0.67
3:M:100:TRP:NE1	3:M:314:THR:OG1	2.22	0.67
3:C:375:GLU:OE2	3:C:391:ARG:NE	2.27	0.67
3:M:375:GLU:OE2	3:M:391:ARG:NE	2.22	0.66
1:A:29:SER:O	1:A:74:ARG:NH1	2.28	0.66
2:B:61:ARG:NH2	2:B:82:ASP:OD2	2.28	0.66
3:M:58:SER:OG	3:M:59:GLU:N	2.29	0.66
2:B:89:GLN:NE2	2:B:96:LEU:HD12	2.11	0.66
3:C:375:GLU:OE2	3:C:391:ARG:CD	2.43	0.66
3:C:406:LEU:HB3	3:C:409:VAL:HB	1.77	0.66
3:C:293:HIS:CG	3:C:294:PRO:HD2	2.30	0.65
3:M:64:HIS:CE1	3:M:296:ARG:HG2	2.31	0.65
1:A:47:TRP:HZ2	1:A:50:GLU:HB2	1.59	0.65
2:B:24:ARG:NH1	2:B:25:THR:HG22	2.12	0.65
3:M:102:THR:HG22	3:M:275:ASN:HD21	1.60	0.64
3:C:74:ALA:HA	3:C:366:THR:HA	1.80	0.63
3:M:31:THR:HG23	3:M:38:GLN:HE22	1.64	0.63
2:L:190:ASN:OD1	2:L:210:ASN:ND2	2.32	0.62
3:M:165:ILE:CG2	5:M:502:ALA:HB2	2.29	0.62
3:M:77:GLY:HA3	5:M:502:ALA:O	2.00	0.62
3:C:387:ILE:O	3:C:391:ARG:CG	2.47	0.62
3:M:165:ILE:HG22	5:M:502:ALA:HB2	1.81	0.62
1:A:47:TRP:CD1	2:B:96:LEU:HD21	2.35	0.61
3:C:122:THR:HA	3:C:129:MET:HA	1.82	0.61
3:M:77:GLY:CA	5:M:502:ALA:O	2.48	0.61
3:M:276:GLU:OE2	3:M:370:TRP:NE1	2.33	0.61
4:M:501:NA:NA	5:M:502:ALA:OXT	1.74	0.61
3:M:74:ALA:HB1	3:M:370:TRP:CD1	2.35	0.61
2:B:193:THR:HG23	2:B:208:SER:HB3	1.83	0.60
3:C:117:ALA:HA	3:C:136:PHE:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:THR:HG23	2:L:208:SER:HB3	1.82	0.60
3:C:309:THR:HA	3:C:313:CYS:HB2	1.83	0.60
3:C:77:GLY:N	3:C:80:ASN:OD1	2.30	0.60
3:M:110:LYS:HZ1	3:M:305:THR:N	1.99	0.60
1:A:1:GLU:OE2	2:L:108:ARG:NH2	2.35	0.60
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.84	0.60
3:C:231:LEU:HB3	3:C:238:ILE:HD11	1.84	0.60
1:A:130:PRO:HB3	1:A:156:TYR:HB3	1.83	0.60
3:M:292:ASP:OD1	3:M:292:ASP:N	2.29	0.60
3:M:45:ALA:HB2	3:M:299:LEU:HB3	1.83	0.60
3:M:292:ASP:OD1	3:M:296:ARG:HD2	2.01	0.59
3:C:369:GLY:O	3:C:373:TYR:HD1	1.85	0.59
3:C:281:SER:O	3:C:373:TYR:HE2	1.85	0.59
3:C:80:ASN:ND2	3:C:274:SER:OG	2.36	0.59
2:B:122:SER:OG	2:B:123:GLU:OE2	2.17	0.59
3:M:109:THR:O	3:M:113:GLU:HG3	2.03	0.59
3:M:60:GLY:HA3	3:M:290:LYS:HA	1.83	0.59
2:B:24:ARG:NH1	2:B:69:THR:HA	2.18	0.58
2:B:89:GLN:HG2	2:B:90:HIS:N	2.16	0.58
2:L:90:HIS:CD2	2:L:97:THR:HG1	2.20	0.58
1:A:3:LYS:HE3	1:A:25:SER:HB2	1.85	0.58
2:L:18:THR:HG22	2:L:76:ASN:HA	1.85	0.58
3:C:20:LEU:HD23	3:C:268:VAL:HG12	1.84	0.58
3:M:60:GLY:HA2	3:M:129:MET:HE1	1.85	0.58
2:B:79:GLN:OE1	2:L:61:ARG:NH1	2.34	0.58
2:L:185:GLU:OE2	2:L:188:ARG:NH2	2.36	0.58
3:M:262:THR:OG1	3:M:263:ALA:N	2.35	0.58
3:M:269:LYS:NZ	3:M:414:ASP:OD2	2.35	0.58
3:M:276:GLU:OE1	3:M:281:SER:OG	2.20	0.58
2:B:24:ARG:CZ	2:B:25:THR:H	2.17	0.58
2:B:90:HIS:CD2	2:B:97:THR:HG1	2.21	0.58
3:C:122:THR:OG1	3:C:127:GLY:O	2.20	0.57
1:H:69:ARG:NH1	1:H:87:SER:O	2.37	0.57
3:M:23:LEU:HG	3:M:278:GLY:HA3	1.87	0.57
3:M:67:ALA:O	3:M:70:THR:OG1	2.22	0.57
3:C:262:THR:OG1	3:C:263:ALA:N	2.37	0.57
2:B:18:THR:HG22	2:B:77:SER:H	1.70	0.56
3:M:57:THR:HA	3:M:290:LYS:HD3	1.86	0.56
3:C:109:THR:O	3:C:113:GLU:HG3	2.05	0.56
3:M:231:LEU:HB3	3:M:238:ILE:HD11	1.88	0.56
2:L:198:HIS:ND1	2:L:200:THR:OG1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:HG3	1:A:160:PRO:HA	1.87	0.55
3:C:37:MET:O	3:C:41:THR:HG22	2.05	0.55
3:C:281:SER:C	3:C:373:TYR:HE2	2.09	0.55
3:C:300:VAL:O	3:C:303:THR:OG1	2.22	0.55
1:H:47:TRP:HZ2	1:H:50:GLU:HB2	1.71	0.55
3:M:320:LEU:HD21	3:M:340:THR:HG22	1.88	0.55
3:C:76:ILE:O	3:C:366:THR:OG1	2.25	0.55
3:M:197:THR:O	3:M:201:ILE:HG12	2.07	0.55
3:C:270:ARG:HA	3:C:270:ARG:NE	2.14	0.55
3:M:116:LEU:HD21	3:M:431:LEU:HB2	1.89	0.55
3:C:281:SER:C	3:C:373:TYR:CE2	2.80	0.54
3:C:239:ILE:HG23	3:C:240:PRO:HD3	1.89	0.54
3:C:293:HIS:CD2	3:C:294:PRO:HD2	2.42	0.54
3:M:24:LEU:O	3:M:28:ILE:HG22	2.07	0.54
2:L:94:TRP:CE3	2:L:94:TRP:HA	2.41	0.54
3:C:387:ILE:CG1	3:C:391:ARG:HE	2.19	0.54
3:M:70:THR:HG22	3:M:208:ILE:HG22	1.89	0.54
3:C:111:TYR:OH	3:C:439:THR:HG22	2.08	0.53
1:H:154:LYS:HB2	1:H:187:THR:HG23	1.90	0.53
3:M:276:GLU:CD	3:M:370:TRP:CZ2	2.78	0.53
3:M:384:THR:O	3:M:387:ILE:HG22	2.09	0.53
3:M:177:ALA:O	3:M:181:ASN:ND2	2.40	0.53
3:C:282:ALA:HB3	3:C:283:PRO:CD	2.37	0.53
3:M:117:ALA:HA	3:M:136:PHE:HE1	1.74	0.53
3:C:219:MET:HE1	3:C:365:SER:HB3	1.90	0.53
3:C:76:ILE:HG23	3:C:362:PHE:CD2	2.44	0.53
3:M:196:PHE:O	3:M:364:TYR:OH	2.27	0.53
3:M:74:ALA:HB2	3:M:369:GLY:HA3	1.91	0.53
3:M:281:SER:HB2	3:M:373:TYR:HD2	1.74	0.53
3:M:260:ILE:HA	3:M:264:ILE:HG12	1.91	0.52
3:C:117:ALA:HA	3:C:136:PHE:CE1	2.45	0.52
3:C:64:HIS:NE2	3:C:290:LYS:O	2.42	0.52
3:C:115:VAL:HG11	3:C:435:VAL:HG23	1.91	0.52
2:B:18:THR:HG22	2:B:76:ASN:HA	1.91	0.52
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.42	0.52
2:B:108:ARG:NH1	2:B:109:ALA:O	2.42	0.52
3:C:31:THR:HG22	3:C:38:GLN:HE22	1.74	0.52
3:C:137:LEU:O	3:C:147:GLY:HA3	2.09	0.52
3:M:34:LEU:HD23	3:M:37:MET:SD	2.50	0.52
3:M:19:MET:SD	3:M:418:GLY:HA2	2.50	0.52
3:M:321:THR:O	3:M:325:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:MET:O	3:C:212:THR:OG1	2.28	0.51
3:C:352:GLY:O	3:C:356:THR:HG22	2.10	0.51
1:A:6:GLU:OE2	1:A:115:GLY:HA3	2.11	0.51
2:B:94:TRP:HA	2:B:94:TRP:CE3	2.45	0.51
3:C:384:THR:O	3:C:387:ILE:HG22	2.10	0.51
3:M:449:GLU:N	3:M:449:GLU:OE2	2.44	0.51
3:C:196:PHE:O	3:C:364:TYR:OH	2.26	0.51
2:B:89:GLN:HE21	2:B:96:LEU:HD12	1.75	0.51
3:M:76:ILE:O	3:M:366:THR:OG1	2.28	0.51
3:M:157:PHE:CD2	3:M:419:ALA:HB1	2.45	0.51
3:C:178:VAL:HG12	3:C:185:ASP:CG	2.32	0.51
3:M:157:PHE:CG	3:M:419:ALA:HB1	2.46	0.51
3:C:328:PHE:CE1	3:C:346:ALA:HB1	2.45	0.50
1:H:27:PHE:CE2	1:H:100:ARG:HD2	2.45	0.50
2:L:40:GLN:NE2	2:L:165:ASP:OD2	2.44	0.50
3:C:64:HIS:HE2	3:C:291:THR:HA	1.76	0.50
1:H:109:GLY:O	2:L:91:ALA:HB2	2.11	0.50
2:L:115:VAL:HA	2:L:135:PHE:O	2.12	0.50
2:L:91:ALA:HA	2:L:96:LEU:HD12	1.94	0.50
3:M:60:GLY:HA2	3:M:129:MET:CE	2.42	0.50
3:M:123:VAL:HG13	3:M:124:ASP:O	2.12	0.50
3:C:134:MET:SD	3:C:134:MET:N	2.85	0.50
3:M:117:ALA:HA	3:M:136:PHE:CE1	2.47	0.49
3:C:56:GLU:OE2	3:C:58:SER:N	2.45	0.49
1:A:198:THR:O	1:A:202:SER:N	2.25	0.49
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.94	0.49
3:M:170:GLN:NE2	5:M:502:ALA:HB1	2.27	0.49
3:M:69:MET:O	3:M:212:THR:OG1	2.29	0.49
3:C:291:THR:OG1	3:C:293:HIS:O	2.23	0.49
1:A:62:TYR:OH	1:A:72:ILE:N	2.30	0.49
2:B:148:TRP:HE1	2:B:177:SER:HG	1.59	0.49
3:C:282:ALA:HB3	3:C:283:PRO:HD3	1.95	0.49
1:H:159:GLU:HG3	1:H:160:PRO:HA	1.94	0.49
3:C:135:TYR:O	3:C:139:LYS:HG2	2.13	0.48
3:M:134:MET:SD	3:M:134:MET:N	2.86	0.48
3:M:185:ASP:OD1	3:M:186:PRO:HD2	2.13	0.48
1:A:52:ALA:O	1:A:74:ARG:NH2	2.46	0.48
3:C:60:GLY:HA3	3:C:290:LYS:HA	1.95	0.48
2:B:96:LEU:H	2:B:96:LEU:CD2	2.27	0.48
3:C:255:GLY:HA3	3:C:258:ALA:HB3	1.96	0.48
1:A:59:GLU:HB2	3:C:405:SER:CA	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:GLN:O	3:C:174:VAL:HG12	2.14	0.48
3:C:248:SER:C	3:C:250:PHE:H	2.16	0.48
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.49	0.48
3:M:133:PRO:HA	3:M:136:PHE:CD2	2.49	0.47
3:C:107:MET:CE	3:C:306:PHE:HB2	2.44	0.47
3:C:116:LEU:HD21	3:C:431:LEU:HB2	1.95	0.47
3:M:176:ASP:OD1	1:H:53:ALA:HB3	2.12	0.47
2:B:185:GLU:OE2	2:B:188:ARG:NH2	2.46	0.47
3:M:309:THR:HA	3:M:313:CYS:HB2	1.96	0.47
2:B:105:GLU:OE1	2:B:173:TYR:OH	2.22	0.47
3:C:49:ALA:CA	3:C:300:VAL:HG22	2.43	0.47
3:M:248:SER:C	3:M:250:PHE:H	2.17	0.47
3:M:167:ASN:HD21	3:M:398:ALA:N	2.12	0.47
3:M:111:TYR:OH	3:M:439:THR:HG22	2.15	0.47
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.75	0.47
1:A:47:TRP:CD1	2:B:96:LEU:CD2	2.98	0.47
1:H:174:VAL:HG12	1:H:192:VAL:HG23	1.97	0.47
3:M:107:MET:CE	3:M:306:PHE:HB2	2.45	0.47
1:A:53:ALA:HB3	3:C:176:ASP:OD1	2.15	0.47
1:A:5:GLU:HB2	1:H:146:MET:HE1	1.97	0.47
2:B:24:ARG:NE	2:B:25:THR:H	2.13	0.46
2:B:17:GLU:O	2:B:78:LEU:HD12	2.14	0.46
3:M:64:HIS:NE2	3:M:290:LYS:O	2.45	0.46
2:L:89:GLN:HE21	2:L:96:LEU:HG	1.79	0.46
3:M:107:MET:HE3	3:M:306:PHE:HB2	1.97	0.46
3:M:412:ILE:O	3:M:415:THR:OG1	2.29	0.46
3:C:74:ALA:HB2	3:C:369:GLY:HA3	1.97	0.46
3:M:224:ILE:HG22	3:M:228:LEU:HD23	1.97	0.46
3:C:68:LEU:HD13	3:C:300:VAL:O	2.16	0.46
3:M:103:ALA:O	3:M:107:MET:N	2.45	0.46
3:C:133:PRO:HA	3:C:136:PHE:CD2	2.51	0.46
3:C:74:ALA:HB1	3:C:370:TRP:CD1	2.51	0.46
1:H:62:TYR:OH	1:H:72:ILE:N	2.33	0.46
3:M:137:LEU:O	3:M:147:GLY:HA3	2.16	0.46
2:B:108:ARG:HG3	2:B:109:ALA:O	2.16	0.46
3:C:118:ILE:HB	3:C:294:PRO:HB3	1.98	0.46
3:M:405:SER:CA	1:H:59:GLU:HB2	2.43	0.46
3:C:114:ALA:HA	3:C:283:PRO:HB3	1.97	0.46
3:C:19:MET:HG3	3:C:20:LEU:HD12	1.98	0.46
3:M:133:PRO:O	3:M:137:LEU:HD23	2.15	0.46
3:M:409:VAL:O	3:M:412:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:422:ILE:O	3:M:426:ILE:HG13	2.16	0.46
1:H:159:GLU:HG3	1:H:160:PRO:CA	2.45	0.46
3:C:260:ILE:HA	3:C:264:ILE:HB	1.98	0.45
2:L:187:GLU:O	2:L:211:ARG:NH2	2.49	0.45
1:H:181:LEU:HD12	1:H:185:LEU:O	2.17	0.45
3:C:98:TRP:CE2	3:C:264:ILE:HG12	2.52	0.45
3:C:72:LEU:HD11	3:C:307:LEU:HD22	1.98	0.45
1:H:39:GLN:OE1	2:L:38:GLN:NE2	2.37	0.45
2:L:39:LYS:NZ	2:L:81:GLU:O	2.35	0.45
3:M:165:ILE:HG23	3:M:273:PHE:CZ	2.52	0.45
3:M:274:SER:HA	5:M:502:ALA:OXT	2.17	0.45
3:M:74:ALA:O	3:M:366:THR:HG23	2.17	0.45
1:H:3:LYS:HE2	1:H:25:SER:OG	2.17	0.45
3:M:188:ILE:O	3:M:192:VAL:HG12	2.17	0.44
3:M:251:ASN:O	3:M:259:LEU:HD23	2.17	0.44
1:A:181:LEU:HB2	1:A:186:TYR:CE1	2.52	0.44
3:C:320:LEU:HD21	3:C:340:THR:HG22	1.99	0.44
3:M:38:GLN:HB3	3:M:107:MET:SD	2.57	0.44
1:H:62:TYR:OH	1:H:72:ILE:HG22	2.18	0.44
2:L:155:ARG:HD3	2:L:179:LEU:HD11	1.99	0.44
3:M:221:VAL:O	3:M:225:LEU:HB2	2.16	0.44
3:M:276:GLU:OE2	3:M:370:TRP:CZ2	2.71	0.44
3:M:72:LEU:HD23	3:M:72:LEU:HA	1.81	0.44
3:C:376:LYS:HD3	3:C:376:LYS:HA	1.80	0.44
3:C:435:VAL:O	3:C:439:THR:N	2.45	0.44
2:L:89:GLN:HG2	2:L:90:HIS:N	2.33	0.44
1:A:159:GLU:HG3	1:A:160:PRO:CA	2.46	0.44
3:M:168:MET:HA	3:M:171:THR:HG22	1.99	0.44
3:C:232:ALA:O	3:C:235:ILE:HG12	2.17	0.44
3:C:356:THR:O	3:C:360:VAL:HG23	2.17	0.44
3:C:76:ILE:CG2	3:C:362:PHE:CD2	3.01	0.44
3:M:257:GLY:O	3:M:260:ILE:HD13	2.17	0.44
3:M:376:LYS:HA	3:M:376:LYS:HD3	1.79	0.44
3:M:165:ILE:HD11	3:M:417:ASN:CG	2.38	0.44
2:B:33:LEU:HD22	2:B:89:GLN:O	2.18	0.44
2:L:94:TRP:HA	2:L:94:TRP:HE3	1.82	0.44
3:C:70:THR:OG1	3:C:212:THR:HG21	2.17	0.43
3:C:98:TRP:CD2	3:C:264:ILE:HG12	2.53	0.43
2:L:19:VAL:HG12	2:L:75:ILE:HB	2.00	0.43
3:M:63:SER:HB3	3:M:66:GLN:HG3	1.99	0.43
3:M:167:ASN:OD1	3:M:397:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:LEU:O	3:C:311:VAL:HB	2.18	0.43
3:M:118:ILE:HG12	3:M:294:PRO:HD3	2.00	0.43
3:C:45:ALA:HB2	3:C:299:LEU:HB3	1.99	0.43
1:H:35:ASP:CG	1:H:47:TRP:HE1	2.20	0.43
2:B:96:LEU:H	2:B:96:LEU:HD23	1.82	0.43
3:C:118:ILE:HD12	3:C:118:ILE:HA	1.88	0.43
3:C:133:PRO:HB3	3:C:424:ASN:HD22	1.83	0.43
3:C:74:ALA:O	3:C:366:THR:HG23	2.18	0.43
3:M:368:LEU:O	3:M:371:SER:HB3	2.18	0.43
2:B:14:SER:HA	2:B:107:LYS:HB2	2.01	0.43
3:C:375:GLU:O	3:C:378:PHE:N	2.52	0.43
1:H:45:LEU:HD23	1:H:45:LEU:HA	1.80	0.43
3:M:69:MET:HG3	3:M:216:VAL:HB	2.00	0.43
3:M:259:LEU:HA	3:M:262:THR:HG23	2.01	0.43
3:M:60:GLY:HA2	3:M:129:MET:SD	2.58	0.43
2:L:33:LEU:HD12	2:L:33:LEU:HA	1.72	0.43
3:C:69:MET:SD	3:C:69:MET:N	2.91	0.43
3:M:317:GLY:O	3:M:321:THR:HG23	2.19	0.43
2:B:24:ARG:HA	2:B:24:ARG:HD2	1.77	0.43
3:M:22:LEU:O	3:M:26:THR:HG23	2.19	0.43
2:B:94:TRP:HA	2:B:94:TRP:HE3	1.84	0.42
3:M:113:GLU:HG2	3:M:428:LEU:HD11	2.01	0.42
3:M:155:ALA:HB1	3:M:377:CYS:O	2.19	0.42
3:M:178:VAL:HG12	3:M:184:VAL:HG22	2.01	0.42
3:M:334:LEU:HD13	3:M:339:LEU:HA	2.01	0.42
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.53	0.42
3:C:123:VAL:HG13	3:C:124:ASP:O	2.18	0.42
3:M:118:ILE:HD12	3:M:118:ILE:HA	1.90	0.42
3:M:356:THR:O	3:M:360:VAL:HG23	2.19	0.42
3:C:33:ARG:HA	3:C:33:ARG:NE	2.35	0.42
2:L:20:THR:OG1	2:L:74:LYS:HE2	2.19	0.42
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.54	0.42
3:M:282:ALA:N	3:M:283:PRO:HD2	2.34	0.42
3:M:64:HIS:HE2	3:M:291:THR:HA	1.84	0.42
3:C:76:ILE:O	3:C:76:ILE:HG22	2.19	0.42
1:A:30:SER:HA	1:A:76:ASP:OD2	2.20	0.42
3:C:208:ILE:O	3:C:212:THR:HG22	2.19	0.42
3:C:296:ARG:HG2	3:C:442:PHE:CE1	2.55	0.42
3:M:218:PHE:HE2	3:M:361:PHE:CE2	2.37	0.42
3:M:28:ILE:O	3:M:32:LEU:HG	2.20	0.42
3:M:440:LYS:HA	3:M:443:ASN:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:CYS:O	1:A:114:TRP:NE1	2.51	0.42
2:B:198:HIS:ND1	2:B:200:THR:OG1	2.48	0.42
2:B:40:GLN:H	2:B:40:GLN:CD	2.21	0.42
3:C:370:TRP:HA	3:C:373:TYR:HB2	2.02	0.42
3:M:194:ALA:HB1	3:M:395:VAL:HG13	2.02	0.42
3:C:178:VAL:HG13	3:C:182:PHE:HD2	1.84	0.42
3:C:167:ASN:HD21	3:C:398:ALA:CA	2.28	0.42
3:C:440:LYS:HA	3:C:440:LYS:HD3	1.60	0.42
2:L:36:TYR:HE1	2:L:89:GLN:HB3	1.85	0.42
1:A:195:PRO:HB2	1:A:198:THR:HG23	2.02	0.41
3:C:197:THR:O	3:C:201:ILE:HG12	2.19	0.41
3:C:368:LEU:O	3:C:371:SER:HB3	2.20	0.41
3:C:440:LYS:HA	3:C:443:ASN:HD21	1.84	0.41
3:M:209:GLY:HA2	3:M:212:THR:HG22	2.02	0.41
3:M:424:ASN:O	3:M:428:LEU:HG	2.20	0.41
3:C:76:ILE:CD1	3:C:76:ILE:N	2.82	0.41
2:L:17:GLU:O	2:L:78:LEU:HD12	2.20	0.41
3:C:76:ILE:HA	3:C:76:ILE:HD12	1.75	0.41
1:A:206:CYS:O	1:A:218:ASP:HA	2.21	0.41
3:C:435:VAL:O	3:C:439:THR:HG23	2.21	0.41
3:M:385:LYS:HG2	3:M:385:LYS:H	1.70	0.41
2:B:4:MET:HA	2:B:25:THR:HA	2.03	0.41
1:H:28:THR:O	1:H:28:THR:OG1	2.39	0.41
1:A:51:ILE:HD13	1:A:74:ARG:HB2	2.03	0.41
3:M:291:THR:OG1	3:M:293:HIS:O	2.34	0.41
3:C:57:THR:HA	3:C:290:LYS:HD3	2.03	0.41
1:H:206:CYS:O	1:H:218:ASP:HA	2.19	0.41
1:A:28:THR:O	1:A:28:THR:OG1	2.36	0.40
3:C:374:GLY:HA2	3:C:377:CYS:SG	2.61	0.40
3:M:31:THR:CG2	3:M:38:GLN:HE22	2.32	0.40
3:C:188:ILE:HA	3:C:188:ILE:HD13	1.91	0.40
3:C:307:LEU:O	3:C:312:VAL:HG23	2.21	0.40
3:M:370:TRP:HA	3:M:373:TYR:HB2	2.03	0.40
1:A:154:LYS:HB2	1:A:187:THR:HG23	2.03	0.40
2:B:195:GLU:HG2	2:B:206:VAL:HG22	2.03	0.40
2:B:36:TYR:HE1	2:B:89:GLN:HB3	1.86	0.40
2:L:122:SER:O	2:L:126:THR:HG23	2.22	0.40
3:M:379:GLU:O	3:M:383:GLY:N	2.43	0.40
2:L:190:ASN:HD21	2:L:212:ALA:HB3	1.86	0.40
3:M:370:TRP:O	3:M:371:SER:C	2.59	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	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17 52
1	H	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	17 52
2	B	211/213 (99%)	204 (97%)	7 (3%)	0	100 100
2	L	211/213 (99%)	204 (97%)	7 (3%)	0	100 100
3	C	422/453 (93%)	388 (92%)	27 (6%)	7 (2%)	9 39
3	M	425/453 (94%)	406 (96%)	18 (4%)	1 (0%)	47 78
All	All	1693/1760 (96%)	1605 (95%)	76 (4%)	12 (1%)	22 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	186	PRO
1	A	53	ALA
1	H	53	ALA
3	C	128	GLU
3	C	129	MET
3	C	328	PHE
1	H	108	ALA
3	C	282	ALA
1	A	108	ALA
3	C	277	ALA
3	C	336	GLY
3	M	336	GLY

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	172/172 (100%)	169 (98%)	3 (2%)	60 81
1	H	172/172 (100%)	168 (98%)	4 (2%)	50 76
2	B	179/179 (100%)	176 (98%)	3 (2%)	60 81
2	L	179/179 (100%)	176 (98%)	3 (2%)	60 81
3	C	315/337 (94%)	303 (96%)	12 (4%)	33 65
3	M	317/337 (94%)	310 (98%)	7 (2%)	52 76
All	All	1334/1376 (97%)	1302 (98%)	32 (2%)	49 75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	95	LEU
1	A	151	CYS
2	B	1	ASP
2	B	24	ARG
2	B	54	LEU
3	M	19	MET
3	M	69	MET
3	M	134	MET
3	M	185	ASP
3	M	225	LEU
3	M	394	PHE
3	M	414	ASP
1	H	74	ARG
1	H	76	ASP
1	H	95	LEU
1	H	154	LYS
3	C	19	MET
3	C	33	ARG
3	C	38	GLN
3	C	69	MET
3	C	76	ILE
3	C	134	MET
3	C	167	ASN
3	C	270	ARG
3	C	350	MET
3	C	391	ARG
3	C	394	PHE

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Mol	Chain	Res	Type
3	C	446	ARG
2	L	1	ASP
2	L	85	SER
2	L	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	297	GLN
3	C	167	ASN
3	C	424	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
5	ALA	M	502	-	2,5,5	0.44	0	2,6,6	0.40	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	ALA	M	502	-	-	0/0/4/4	-

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.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	502	ALA	7	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, 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	214/214 (100%)	0.49	6 (2%) 53 41	60, 83, 115, 141	0
1	H	214/214 (100%)	0.29	3 (1%) 75 66	62, 84, 118, 156	0
2	B	213/213 (100%)	0.23	2 (0%) 84 78	63, 88, 123, 174	0
2	L	213/213 (100%)	0.32	3 (1%) 75 66	62, 88, 122, 144	0
3	C	428/453 (94%)	0.49	36 (8%) 11 7	88, 129, 174, 225	0
3	M	431/453 (95%)	0.46	26 (6%) 21 14	81, 115, 156, 190	0
All	All	1713/1760 (97%)	0.40	76 (4%) 34 24	60, 103, 155, 225	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	130	ALA	6.7
3	M	137	LEU	5.4
3	C	293	HIS	5.0
3	M	444	GLU	5.0
3	M	125	ASP	4.8
3	C	53	HIS	4.1
3	M	121	ARG	4.1
3	C	121	ARG	4.0
3	C	294	PRO	4.0
3	M	430	LEU	4.0
3	M	408	LEU	3.9
3	M	126	ASN	3.8
1	H	99	THR	3.7
3	M	131	GLY	3.7
3	C	131	GLY	3.6
3	C	122	THR	3.6
3	M	447	LYS	3.5
3	M	388	ARG	3.4
2	L	25	THR	3.4

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Mol	Chain	Res	Type	RSRZ
3	M	122	THR	3.4
1	A	99	THR	3.3
3	M	446	ARG	3.2
2	B	1	ASP	3.2
3	C	110	LYS	3.2
3	M	33	ARG	3.2
1	A	101	THR	3.2
3	C	113	GLU	3.1
3	M	431	LEU	3.1
1	A	29	SER	3.0
3	M	443	ASN	3.0
3	C	302	MET	2.9
3	C	448	ASN	2.8
3	C	277	ALA	2.8
3	M	29	PHE	2.8
3	M	434	VAL	2.8
3	C	39	ILE	2.8
3	C	305	THR	2.7
3	C	386	GLY	2.7
3	C	114	ALA	2.6
3	C	111	TYR	2.6
3	C	281	SER	2.6
3	C	36	PHE	2.5
3	C	289	ALA	2.5
3	M	440	LYS	2.5
1	A	34	MET	2.5
3	M	127	GLY	2.5
3	C	280	GLY	2.5
3	M	436	VAL	2.4
2	L	40	GLN	2.4
3	M	441	ALA	2.4
3	C	303	THR	2.4
3	M	445	ILE	2.4
3	C	126	ASN	2.3
3	M	32	LEU	2.3
3	M	429	LEU	2.3
1	A	108	ALA	2.3
3	C	42	LEU	2.3
3	C	297	GLN	2.3
1	H	35	ASP	2.3
3	C	286	ALA	2.3
1	A	4	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	4	LEU	2.2
3	C	115	VAL	2.2
3	M	120	TYR	2.2
3	C	292	ASP	2.2
2	L	1	ASP	2.2
3	C	382	ILE	2.1
3	C	287	ALA	2.1
3	C	120	TYR	2.1
3	C	307	LEU	2.1
3	C	304	GLY	2.1
3	C	125	ASP	2.1
2	B	69	THR	2.0
3	M	442	PHE	2.0
3	C	299	LEU	2.0
3	C	52	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
4	NA	M	501	1/1	0.81	0.06	106,106,106,106	0
5	ALA	M	502	6/6	0.92	0.29	118,123,125,129	0

6.5 Other polymers (i)

There are no such residues in this entry.