Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:32 PM GMT

PDB ID	:	3ZR4
Title	:	STRUCTURAL EVIDENCE FOR AMMONIA TUNNELING ACROSS THE (BETA-ALPHA)8 BARREL OF THE IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE BIENZYME COMPLEX
Authors	:	Vega, M.C.; Kuper, J.; Haeger, M.C.; Mohrlueder, J.; Marquardt, S.; Sterner, R.; Wilmanns, M.
Deposited on	:	2011-06-13
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

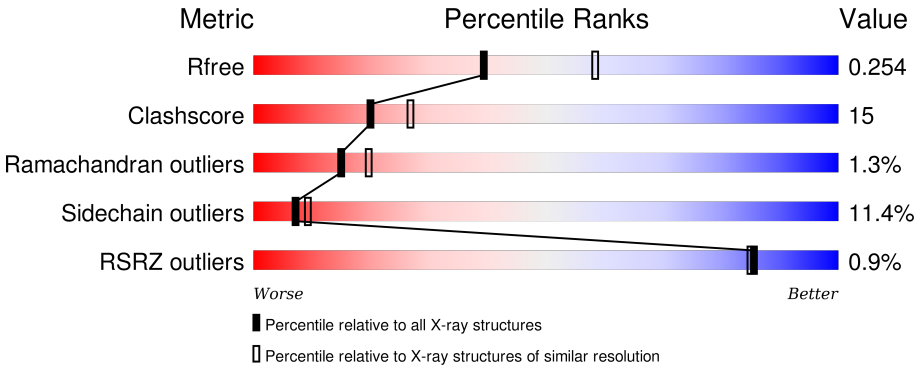
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	64% 28%
1	C	253	71% 23%
1	E	253	59% 30% 7%
2	B	201	59% 35% 6%
2	D	201	62% 31% 7%

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Mol	Chain	Length	Quality of chain
2	F	201	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10728 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.

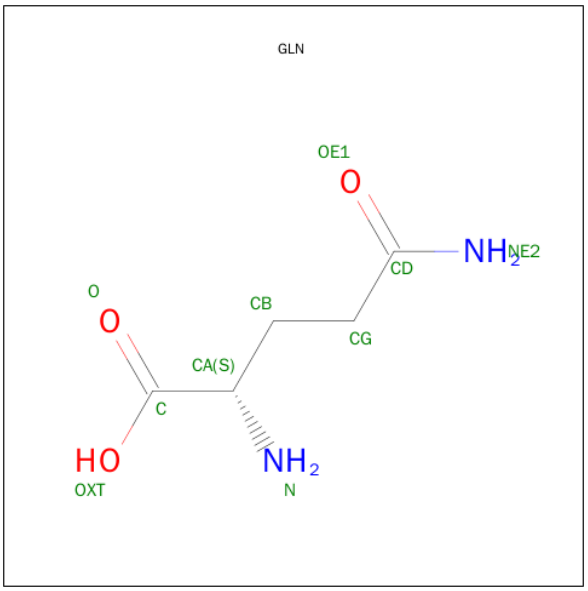
- Molecule 1 is a protein called IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1862	1188	314	354	6			
1	C	244	Total	C	N	O	S	0	0	0
			1875	1196	317	356	6			
1	E	244	Total	C	N	O	S	0	0	0
			1877	1197	317	357	6			

- Molecule 2 is a protein called IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISH.

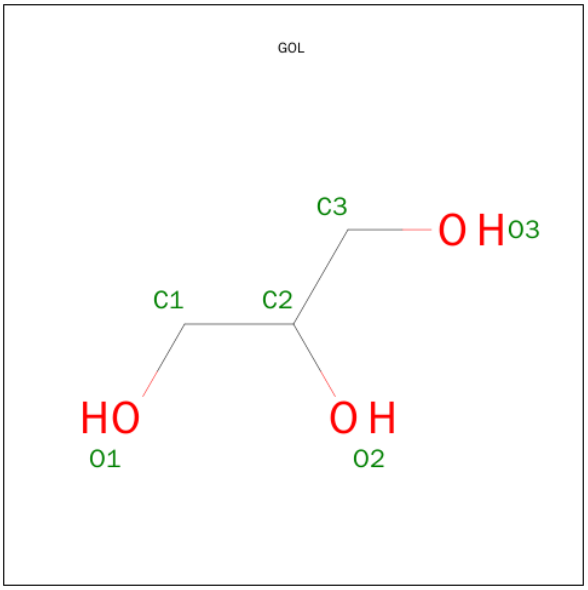
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	201	Total	C	N	O	S	0	0	1
			1616	1029	285	294	8			
2	D	201	Total	C	N	O	S	0	0	1
			1616	1029	285	294	8			
2	F	201	Total	C	N	O	S	0	0	1
			1616	1029	285	294	8			

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	2	3		
3	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

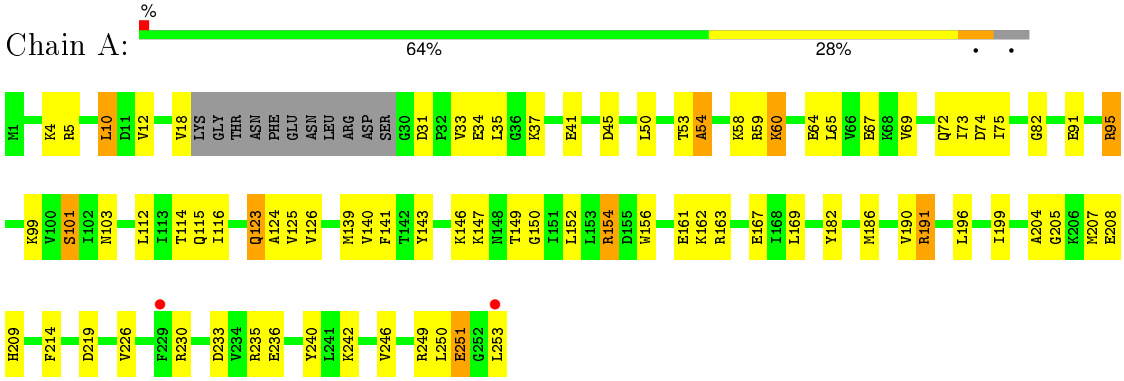
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	43	Total O 43 43	0	0
5	C	43	Total O 43 43	0	0
5	D	42	Total O 42 42	0	0
5	E	13	Total O 13 13	0	0
5	F	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

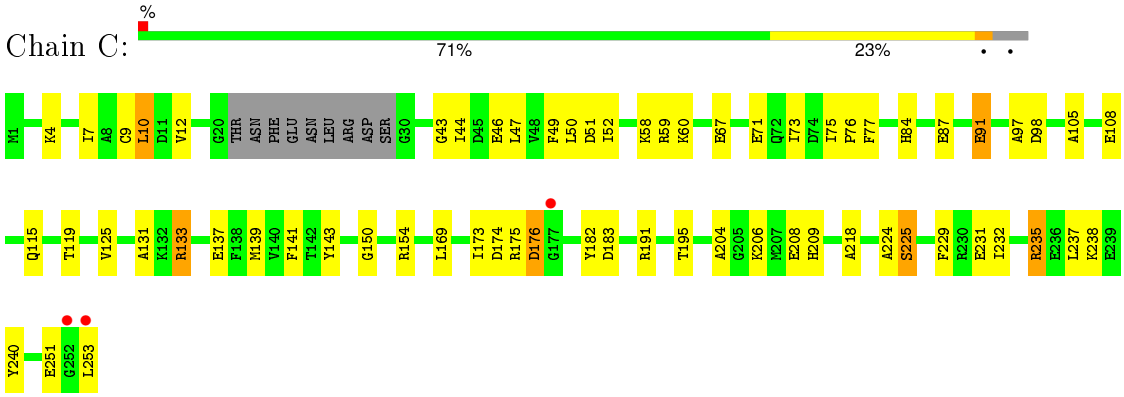
• Molecule 1: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISF

Chain A:



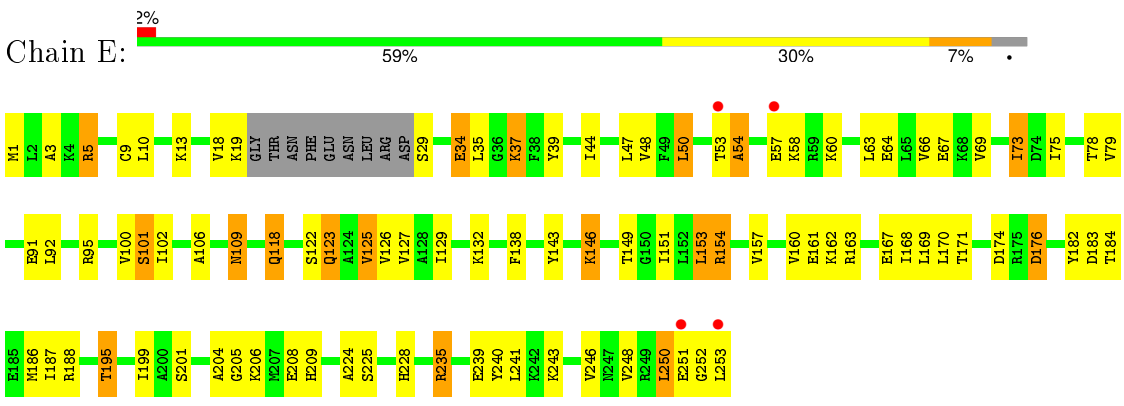
• Molecule 1: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISF

Chain C:



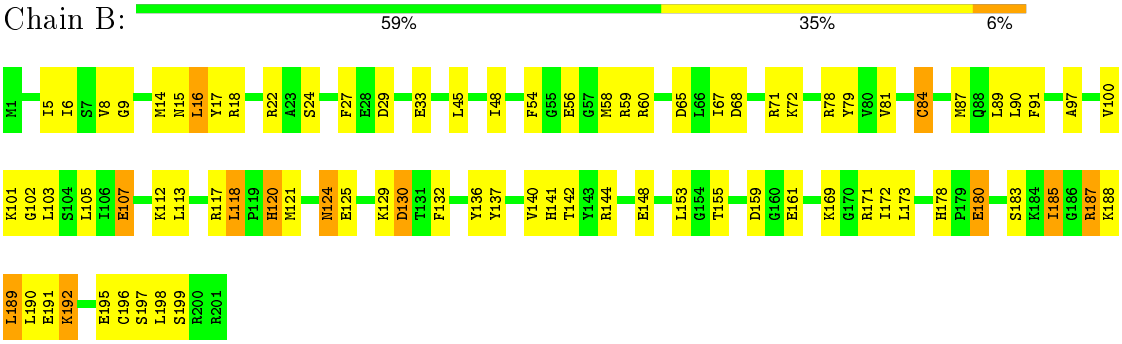
• Molecule 1: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISF

Chain E:



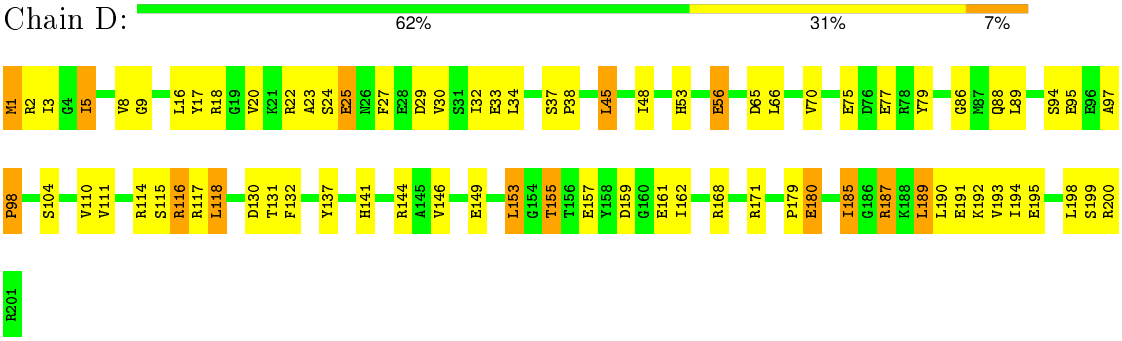
• Molecule 2: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISH

Chain B:



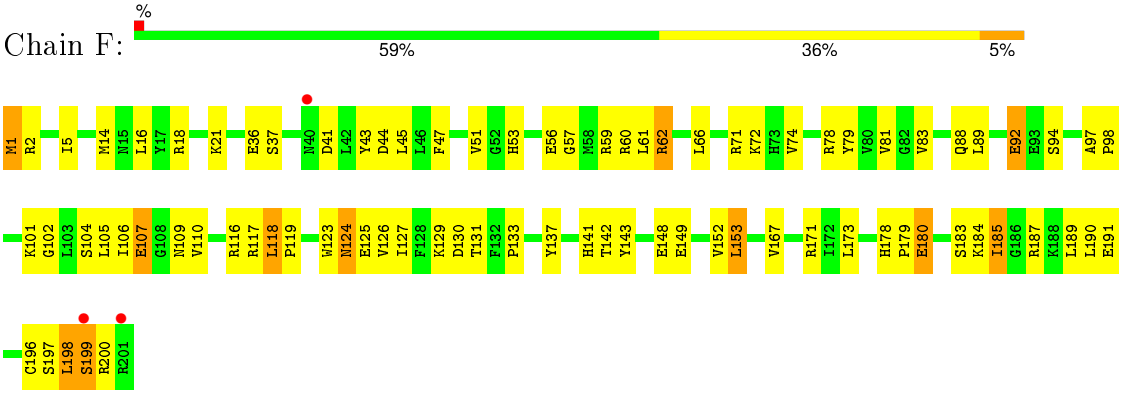
• Molecule 2: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISH

Chain D:



• Molecule 2: IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE SUBUNIT HISH

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	85.40Å 85.40Å 171.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.96 – 2.41 55.95 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.0 (55.96-2.41) 96.1 (55.95-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.194 , 0.258 0.192 , 0.254	Depositor DCC
R_{free} test set	4335 reflections (9.14%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.6	EDS
Estimated twinning fraction	0.507 for H, K, L 0.493 for -H-K, K, -L 0.021 for -h,-k,l 0.477 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for -H-K, K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 51681 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10728	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.60	0/1887	0.70	0/2542
1	C	0.56	0/1900	0.72	0/2558
1	E	0.59	0/1902	0.70	0/2561
2	B	0.67	1/1650 (0.1%)	0.77	1/2220 (0.0%)
2	D	0.62	0/1650	0.76	0/2220
2	F	0.62	0/1650	0.75	2/2220 (0.1%)
All	All	0.61	1/10639 (0.0%)	0.73	3/14321 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	84	CYS	CB-SG	7.31	1.94	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	153	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	189	LEU	CA-CB-CG	5.21	127.28	115.30
2	F	189	LEU	CA-CB-CG	5.04	126.90	115.30

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	1862	0	1909	58	0
1	C	1875	0	1925	42	0
1	E	1877	0	1927	60	0
2	B	1616	0	1611	63	0
2	D	1616	0	1611	56	0
2	F	1616	0	1611	46	0
3	B	10	0	7	1	0
3	D	10	0	7	0	0
4	A	6	0	8	0	0
4	B	12	0	16	1	0
4	C	6	0	8	2	0
4	D	6	0	8	0	0
4	E	12	0	16	1	0
5	A	52	0	0	2	0
5	B	43	0	0	1	0
5	C	43	0	0	0	0
5	D	42	0	0	3	0
5	E	13	0	0	2	0
5	F	11	0	0	0	0
All	All	10728	0	10664	313	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 15.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ARG:HG3	2:D:116:ARG:HH11	1.17	1.05
2:B:124:ASN:HD22	2:B:125:GLU:H	1.07	1.00
2:B:121:MET:HG3	2:B:140:VAL:HG22	1.43	1.00
1:E:184:THR:O	1:E:188:ARG:HG3	1.66	0.95
1:A:123:GLN:H	1:A:123:GLN:HE21	0.98	0.93
2:F:16:LEU:HA	2:F:180:GLU:HG2	1.52	0.91
2:F:187:ARG:NH1	2:F:191:GLU:OE2	2.04	0.91
2:F:81:VAL:HG22	2:F:173:LEU:HB2	1.58	0.84
1:E:123:GLN:HE21	1:E:123:GLN:H	1.26	0.83
2:B:120:HIS:HD2	2:B:141:HIS:NE2	1.75	0.83
1:C:133:ARG:NH2	1:C:174:ASP:HB2	1.95	0.82
2:B:124:ASN:HD22	2:B:125:GLU:N	1.80	0.80
1:E:9:CYS:HB3	1:E:224:ALA:HB2	1.63	0.80
2:F:57:GLY:O	2:F:61:LEU:HG	1.82	0.79
2:F:62:ARG:HG3	2:F:62:ARG:HH11	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:LEU:HA	2:D:180:GLU:HG2	1.67	0.77
1:C:195:THR:O	2:D:117:ARG:HD3	1.85	0.77
2:D:116:ARG:CG	2:D:116:ARG:HH11	1.97	0.76
2:D:187:ARG:HH11	2:D:187:ARG:CG	1.99	0.75
2:F:141:HIS:HD2	2:F:143:TYR:O	1.70	0.75
2:D:66:LEU:O	2:D:70:VAL:HG23	1.86	0.75
1:C:87:GLU:O	1:C:91:GLU:HG3	1.86	0.74
2:F:62:ARG:CG	2:F:62:ARG:HH11	2.01	0.73
2:D:187:ARG:HH11	2:D:187:ARG:HG3	1.52	0.73
2:B:71:ARG:HH22	2:B:103:LEU:HA	1.54	0.73
2:D:116:ARG:HG3	2:D:116:ARG:NH1	1.96	0.71
2:F:133:PRO:HB2	2:F:185:ILE:HD11	1.71	0.71
2:D:8:VAL:HG23	2:D:9:GLY:N	2.02	0.71
1:A:123:GLN:H	1:A:123:GLN:NE2	1.82	0.71
1:E:161:GLU:OE2	2:F:117:ARG:NH2	2.24	0.71
2:B:16:LEU:HA	2:B:180:GLU:HG2	1.74	0.70
1:A:53:THR:O	1:A:54:ALA:O	2.08	0.70
2:F:16:LEU:CA	2:F:180:GLU:HG2	2.20	0.70
2:F:119:PRO:HB3	2:F:142:THR:OG1	1.92	0.70
2:D:132:PHE:CE1	2:D:192:LYS:HG3	2.27	0.70
2:B:59:ARG:HH21	2:B:60:ARG:HD3	1.57	0.69
1:A:10:LEU:HD13	1:A:35:LEU:HD23	1.75	0.69
2:B:33:GLU:HG2	1:E:243:LYS:HG2	1.75	0.69
2:D:8:VAL:CG2	2:D:9:GLY:N	2.56	0.69
1:E:48:VAL:HG22	1:E:78:THR:HB	1.74	0.69
1:A:60:LYS:HD3	1:A:60:LYS:O	1.93	0.69
1:C:133:ARG:HH22	1:C:174:ASP:HB2	1.56	0.69
2:D:130:ASP:OD2	2:D:131:THR:OG1	2.11	0.68
2:B:112:LYS:HE2	2:B:118:LEU:HD23	1.74	0.68
2:F:81:VAL:HA	2:F:173:LEU:O	1.93	0.67
1:E:154:ARG:NH1	1:E:154:ARG:H	1.93	0.67
1:A:123:GLN:N	1:A:123:GLN:HE21	1.83	0.65
1:E:241:LEU:O	1:E:246:VAL:HB	1.97	0.65
2:D:137:TYR:CZ	2:D:185:ILE:HD12	2.31	0.64
1:C:173:ILE:O	1:C:176:ASP:HB2	1.97	0.64
2:F:183:SER:OG	2:F:184:LYS:N	2.30	0.64
1:C:59:ARG:NH2	1:C:87:GLU:HG3	2.12	0.64
1:A:191:ARG:HD3	1:A:191:ARG:O	1.98	0.64
2:D:159:ASP:OD1	5:D:2024:HOH:O	2.15	0.63
2:D:1:MET:HE3	2:D:198:LEU:HD12	1.80	0.63
1:E:126:VAL:HG22	1:E:167:GLU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HE3	1:A:150:GLY:HA2	1.80	0.62
1:A:233:ASP:HB3	1:A:236:GLU:HB2	1.80	0.62
1:C:235:ARG:CG	1:C:235:ARG:HH11	2.13	0.62
2:D:53:HIS:O	2:D:56:GLU:O	2.16	0.62
2:B:79:TYR:CE2	2:B:171:ARG:NH1	2.68	0.61
2:F:124:ASN:HD22	2:F:125:GLU:N	1.98	0.61
2:B:121:MET:CG	2:B:140:VAL:HG22	2.24	0.61
2:B:8:VAL:CG2	2:B:9:GLY:N	2.64	0.61
2:D:27:PHE:HZ	2:D:195:GLU:HG3	1.65	0.61
1:A:69:VAL:HG13	1:A:73:ILE:HG13	1.82	0.61
1:E:205:GLY:H	1:E:209:HIS:HD2	1.47	0.61
2:B:137:TYR:OH	2:B:185:ILE:HD13	2.00	0.60
1:A:12:VAL:HG21	1:A:65:LEU:CD2	2.31	0.60
2:F:101:LYS:HD3	2:F:102:GLY:O	2.01	0.60
1:C:7:ILE:HG12	1:C:46:GLU:HB2	1.82	0.59
1:E:39:TYR:O	1:E:44:ILE:HB	2.02	0.59
2:D:116:ARG:NH2	5:D:2024:HOH:O	1.97	0.59
2:B:187:ARG:HD3	2:B:191:GLU:OE2	2.02	0.59
1:E:129:ILE:HG13	1:E:168:ILE:HG23	1.85	0.59
2:B:8:VAL:HG23	2:B:9:GLY:N	2.16	0.59
2:D:48:ILE:O	2:D:86:GLY:HA3	2.03	0.59
2:B:16:LEU:CA	2:B:180:GLU:HG2	2.33	0.58
2:B:137:TYR:OH	2:B:185:ILE:CD1	2.52	0.58
1:A:58:LYS:HZ3	1:A:82:GLY:HA3	1.68	0.58
1:A:116:ILE:CG2	1:A:125:VAL:HG22	2.34	0.58
1:E:170:LEU:HD21	1:E:186:MET:HG2	1.83	0.58
2:F:118:LEU:HD22	2:F:118:LEU:H	1.69	0.58
2:F:62:ARG:CG	2:F:62:ARG:NH1	2.64	0.57
2:F:141:HIS:CD2	2:F:143:TYR:O	2.57	0.57
1:C:150:GLY:HA3	4:C:1254:GOL:H2	1.86	0.57
1:C:133:ARG:NE	1:C:133:ARG:H	2.04	0.56
1:E:127:VAL:HG12	1:E:129:ILE:HG12	1.87	0.56
1:C:10:LEU:HD12	1:C:49:PHE:CE2	2.41	0.56
2:B:196:CYS:SG	5:B:2043:HOH:O	2.58	0.56
2:B:87:MET:O	2:B:90:LEU:HB2	2.04	0.56
2:F:118:LEU:CD2	2:F:118:LEU:H	2.19	0.56
1:A:101:SER:HA	1:A:126:VAL:O	2.05	0.56
1:E:122:SER:HA	1:E:125:VAL:HG23	1.87	0.56
2:D:194:ILE:O	2:D:198:LEU:HD13	2.06	0.56
1:C:4:LYS:HE3	1:C:218:ALA:O	2.05	0.56
2:D:88:GLN:NE2	5:D:2021:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:ARG:O	2:D:191:GLU:HG3	2.07	0.55
1:E:206:LYS:NZ	1:E:209:HIS:CE1	2.75	0.55
1:C:237:LEU:O	1:C:240:TYR:HB3	2.06	0.55
1:C:84:HIS:HA	1:C:105:ALA:HB2	1.88	0.55
1:C:115:GLN:O	1:C:119:THR:OG1	2.22	0.55
2:B:84:CYS:SG	2:B:178:HIS:CE1	3.00	0.55
1:C:195:THR:O	2:D:117:ARG:CD	2.54	0.54
2:D:17:TYR:CD2	2:D:34:LEU:HD21	2.42	0.54
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.71	0.54
2:B:79:TYR:HE2	2:B:171:ARG:NH1	2.05	0.54
2:D:16:LEU:CA	2:D:180:GLU:HG2	2.36	0.54
1:A:12:VAL:HG21	1:A:65:LEU:HD21	1.89	0.54
1:A:99:LYS:HB3	1:A:124:ALA:HA	1.89	0.54
2:B:105:LEU:O	2:B:169:LYS:NZ	2.36	0.54
2:F:2:ARG:HG2	2:F:43:TYR:CD1	2.43	0.54
1:C:182:TYR:CZ	1:C:204:ALA:HB2	2.43	0.54
1:A:205:GLY:H	1:A:209:HIS:HD2	1.56	0.54
1:C:133:ARG:HA	1:C:137:GLU:O	2.07	0.53
2:B:71:ARG:HH22	2:B:103:LEU:CA	2.20	0.53
1:E:48:VAL:HG12	1:E:50:LEU:HD12	1.89	0.53
2:B:185:ILE:HA	2:B:188:LYS:CE	2.38	0.53
2:F:37:SER:HA	2:F:66:LEU:HD21	1.89	0.53
2:D:179:PRO:HD2	2:D:180:GLU:OE2	2.08	0.53
1:A:33:VAL:HG11	1:A:72:GLN:HE21	1.74	0.53
2:B:101:LYS:HD3	2:B:102:GLY:O	2.09	0.53
1:E:3:ALA:HB3	2:F:123:TRP:HB2	1.90	0.53
1:E:183:ASP:O	1:E:187:ILE:HG13	2.09	0.53
1:C:77:PHE:CZ	1:C:97:ALA:HA	2.43	0.53
2:F:43:TYR:O	2:F:78:ARG:HD2	2.09	0.53
1:E:47:LEU:HG	1:E:75:ILE:HD11	1.90	0.52
1:E:169:LEU:HA	1:E:199:ILE:HB	1.91	0.52
2:B:56:GLU:OE2	2:B:60:ARG:NH2	2.43	0.52
1:E:169:LEU:HD22	5:E:2006:HOH:O	2.09	0.52
1:C:175:ARG:HG3	1:C:183:ASP:HB2	1.92	0.52
1:C:206:LYS:HG2	1:C:209:HIS:CE1	2.45	0.52
1:A:191:ARG:NH2	1:A:219:ASP:OD1	2.43	0.52
1:C:108:GLU:OE2	1:C:143:TYR:OH	2.24	0.52
2:F:1:MET:HE3	2:F:198:LEU:HD13	1.93	0.51
2:F:124:ASN:HD22	2:F:125:GLU:H	1.58	0.51
2:B:72:LYS:HD3	4:B:1202:GOL:H11	1.92	0.51
1:E:53:THR:HG22	1:E:54:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:CE	1:A:150:GLY:HA2	2.41	0.51
1:C:150:GLY:CA	4:C:1254:GOL:H2	2.40	0.51
2:B:107:GLU:H	2:B:107:GLU:CD	2.14	0.51
1:C:46:GLU:HG2	1:C:76:PRO:HB2	1.92	0.51
2:B:185:ILE:HG12	2:B:188:LYS:HE3	1.92	0.51
2:F:14:MET:O	2:F:18:ARG:HG3	2.10	0.51
2:B:33:GLU:HB3	1:E:243:LYS:O	2.11	0.50
1:A:4:LYS:HG3	1:A:246:VAL:HG13	1.93	0.50
2:D:153:LEU:HG	2:D:168:ARG:HB2	1.93	0.50
2:F:16:LEU:HD22	2:F:83:VAL:HG11	1.93	0.50
2:B:58:MET:SD	2:B:89:LEU:HD22	2.52	0.50
2:B:192:LYS:HE3	2:B:195:GLU:OE1	2.10	0.50
1:C:71:GLU:HA	2:D:18:ARG:NE	2.27	0.50
1:A:156:TRP:HA	1:A:156:TRP:CE3	2.47	0.50
1:A:191:ARG:HD3	1:A:191:ARG:C	2.31	0.50
2:B:185:ILE:HA	2:B:188:LYS:HE2	1.92	0.50
2:D:115:SER:HB3	2:D:118:LEU:HD13	1.93	0.50
2:B:84:CYS:HB2	2:B:178:HIS:CE1	2.47	0.50
1:E:53:THR:HB	1:E:58:LYS:HB2	1.94	0.50
2:D:1:MET:HB3	2:D:30:VAL:HG23	1.92	0.49
1:E:206:LYS:HZ2	1:E:209:HIS:CE1	2.29	0.49
2:B:91:PHE:O	2:B:102:GLY:HA3	2.13	0.49
1:E:208:GLU:HG3	1:E:240:TYR:OH	2.13	0.49
1:E:13:LYS:HB3	1:E:18:VAL:HG21	1.94	0.49
2:F:197:SER:C	2:F:199:SER:H	2.16	0.49
1:A:67:GLU:OE1	1:A:95:ARG:NH2	2.45	0.49
1:A:249:ARG:HG3	2:B:136:TYR:HB2	1.95	0.49
1:A:37:LYS:O	1:A:41:GLU:HG3	2.12	0.48
1:A:112:LEU:O	1:A:116:ILE:HG13	2.13	0.48
2:B:68:ASP:O	2:B:72:LYS:HG3	2.13	0.48
1:A:161:GLU:HA	1:A:196:LEU:HD11	1.95	0.48
1:E:79:VAL:O	1:E:100:VAL:HA	2.14	0.48
1:E:53:THR:HG22	1:E:54:ALA:H	1.78	0.48
2:D:45:LEU:HD11	2:D:193:VAL:HG12	1.94	0.48
1:C:235:ARG:NH1	1:C:235:ARG:CG	2.74	0.48
2:D:3:ILE:HD12	2:D:32:ILE:CD1	2.44	0.48
1:A:141:PHE:HA	1:A:147:LYS:O	2.13	0.48
1:C:229:PHE:HB2	1:C:231:GLU:HG3	1.95	0.48
1:A:10:LEU:HD23	1:A:10:LEU:N	2.29	0.48
1:A:33:VAL:HG22	1:A:69:VAL:HA	1.96	0.48
1:C:133:ARG:HH22	1:C:174:ASP:CB	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:SER:HB2	2:D:38:PRO:HD2	1.95	0.47
2:D:27:PHE:CZ	2:D:195:GLU:HG3	2.49	0.47
2:B:78:ARG:HH11	2:B:78:ARG:HG2	1.78	0.47
1:E:171:THR:HA	1:E:201:SER:O	2.14	0.47
1:E:101:SER:HA	1:E:126:VAL:O	2.14	0.47
1:E:69:VAL:HG13	1:E:73:ILE:HG13	1.95	0.47
1:A:74:ASP:OD1	2:B:183:SER:HA	2.14	0.47
1:C:59:ARG:NH2	1:C:87:GLU:OE2	2.47	0.47
2:D:155:THR:HG22	2:D:162:ILE:HG12	1.96	0.47
2:B:84:CYS:SG	3:B:1205:GLN:HG3	2.55	0.47
2:B:6:ILE:HD12	2:B:48:ILE:HG12	1.96	0.47
1:C:141:PHE:HB2	1:C:173:ILE:HD11	1.97	0.47
2:F:5:ILE:HG12	2:F:47:PHE:HB2	1.96	0.47
2:B:172:ILE:O	2:B:173:LEU:HD23	2.14	0.47
2:F:59:ARG:NH2	2:F:60:ARG:HE	2.13	0.47
2:F:79:TYR:CE1	2:F:171:ARG:HD2	2.49	0.47
2:D:3:ILE:HB	2:D:32:ILE:HD13	1.97	0.46
1:E:206:LYS:H	1:E:209:HIS:CD2	2.33	0.46
2:B:113:LEU:HB2	2:B:118:LEU:HD11	1.97	0.46
1:A:156:TRP:HE3	1:A:156:TRP:HA	1.81	0.46
1:A:67:GLU:CD	1:A:95:ARG:NH2	2.69	0.46
2:B:132:PHE:CD1	2:B:189:LEU:HD22	2.50	0.46
2:F:133:PRO:HB2	2:F:185:ILE:CD1	2.43	0.46
2:D:137:TYR:OH	2:D:185:ILE:CD1	2.64	0.46
2:F:106:ILE:HD13	2:F:167:VAL:CG1	2.46	0.46
2:D:94:SER:HB2	2:D:110:VAL:HB	1.98	0.46
2:F:126:VAL:O	2:F:127:ILE:HD13	2.15	0.46
1:C:9:CYS:O	1:C:224:ALA:CB	2.64	0.46
1:A:250:LEU:O	1:A:251:GLU:O	2.34	0.46
2:B:14:MET:O	2:B:18:ARG:HG3	2.16	0.46
1:A:186:MET:O	1:A:190:VAL:HG23	2.16	0.46
1:E:235:ARG:HH21	1:E:250:LEU:HD22	1.81	0.46
2:B:97:ALA:HB1	2:B:100:VAL:HB	1.97	0.46
2:D:37:SER:HB2	2:D:38:PRO:CD	2.46	0.46
1:A:242:LYS:HD2	1:A:250:LEU:HD12	1.99	0.45
1:E:10:LEU:HD22	1:E:228:HIS:CE1	2.52	0.45
1:A:167:GLU:OE2	1:A:199:ILE:CG1	2.64	0.45
2:F:88:GLN:HG2	2:F:110:VAL:HG11	1.96	0.45
2:F:129:LYS:NZ	2:F:152:VAL:HB	2.32	0.45
1:E:54:ALA:HB3	1:E:57:GLU:HB2	1.98	0.45
1:E:1:MET:N	2:F:124:ASN:HD21	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ILE:HD12	1:E:106:ALA:HB2	1.99	0.45
1:C:191:ARG:NE	1:C:191:ARG:HA	2.31	0.45
1:A:116:ILE:HB	1:A:125:VAL:CG2	2.46	0.45
1:C:77:PHE:O	1:C:98:ASP:HB2	2.16	0.45
2:D:23:ALA:HA	2:D:187:ARG:HH12	1.81	0.45
2:B:18:ARG:HB3	2:B:22:ARG:NH2	2.32	0.45
1:C:52:ILE:O	1:C:52:ILE:HG13	2.16	0.45
1:E:66:VAL:HG21	1:E:92:LEU:HD22	1.99	0.45
2:B:137:TYR:CZ	2:B:185:ILE:HD12	2.51	0.44
1:C:206:LYS:HE3	1:C:208:GLU:HB3	1.99	0.44
2:D:22:ARG:HA	2:D:25:GLU:OE2	2.18	0.44
1:E:118:GLN:HA	1:E:118:GLN:HE21	1.82	0.44
2:F:101:LYS:HE3	2:F:104:SER:OG	2.18	0.44
1:A:31:ASP:HB3	1:A:34:GLU:HB2	2.00	0.44
1:A:73:ILE:HG22	1:A:75:ILE:H	1.82	0.44
1:E:34:GLU:O	1:E:37:LYS:HB2	2.18	0.44
2:B:137:TYR:CZ	2:B:185:ILE:CD1	3.01	0.44
2:F:79:TYR:CZ	2:F:196:CYS:HB3	2.52	0.44
1:E:109:ASN:ND2	1:E:109:ASN:C	2.69	0.44
1:E:5:ARG:HD3	5:E:2001:HOH:O	2.17	0.44
2:F:74:VAL:HG21	2:F:105:LEU:HD22	2.00	0.44
2:D:95:GLU:OE1	2:D:111:VAL:HG13	2.17	0.44
1:C:131:ALA:HA	1:C:139:MET:O	2.17	0.44
1:A:207:MET:HB3	1:A:240:TYR:CD2	2.53	0.44
1:A:208:GLU:HA	1:A:240:TYR:OH	2.17	0.44
1:A:103:ASN:HB3	5:A:2026:HOH:O	2.17	0.43
1:A:219:ASP:OD2	2:B:117:ARG:NH2	2.42	0.43
1:E:39:TYR:HB3	1:E:47:LEU:HD21	1.99	0.43
1:A:91:GLU:O	1:A:95:ARG:HB2	2.17	0.43
2:D:23:ALA:HA	2:D:187:ARG:NH1	2.34	0.43
2:F:178:HIS:HA	2:F:179:PRO:HD2	1.86	0.43
1:C:12:VAL:O	1:C:51:ASP:HA	2.18	0.43
1:E:182:TYR:CZ	1:E:204:ALA:HB2	2.53	0.43
1:A:114:THR:OG1	1:A:163:ARG:O	2.33	0.43
2:B:118:LEU:HG	2:B:142:THR:HG23	2.00	0.43
2:F:2:ARG:HB3	2:F:44:ASP:H	1.82	0.43
1:A:242:LYS:HD2	1:A:250:LEU:CD1	2.49	0.43
2:D:79:TYR:CE1	2:D:171:ARG:HG2	2.54	0.43
1:C:206:LYS:HA	1:C:232:ILE:HD11	2.01	0.42
2:D:132:PHE:HE1	2:D:192:LYS:HG3	1.79	0.42
2:B:24:SER:HA	2:B:27:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ARG:NH1	4:E:1254:GOL:O3	2.37	0.42
2:B:81:VAL:HA	2:B:173:LEU:O	2.19	0.42
2:D:116:ARG:H	2:D:116:ARG:HH11	1.66	0.42
1:E:149:THR:OG1	1:E:151:ILE:HD12	2.19	0.42
2:B:81:VAL:HG22	2:B:173:LEU:HB2	2.00	0.42
2:B:54:PHE:HB3	2:B:97:ALA:HB2	2.01	0.42
2:B:71:ARG:NH2	2:B:103:LEU:HB3	2.34	0.42
2:D:17:TYR:CD2	2:D:34:LEU:CD2	3.03	0.42
1:E:109:ASN:HD22	1:E:109:ASN:C	2.22	0.42
2:D:187:ARG:NH1	2:D:187:ARG:CG	2.67	0.42
2:F:137:TYR:CE2	2:F:185:ILE:HG23	2.55	0.42
1:E:246:VAL:HG12	1:E:248:VAL:HG13	2.02	0.42
1:A:5:ARG:HA	1:A:45:ASP:OD2	2.20	0.42
1:C:47:LEU:HG	1:C:75:ILE:HD11	2.01	0.42
1:A:4:LYS:HB3	1:A:214:PHE:CE1	2.54	0.42
1:C:43:GLY:O	1:C:238:LYS:NZ	2.49	0.42
2:D:2:ARG:NH1	2:D:33:GLU:OE2	2.50	0.42
1:E:239:GLU:HG2	1:E:250:LEU:HD11	2.02	0.41
1:A:143:TYR:O	1:A:146:LYS:HB2	2.19	0.41
2:B:144:ARG:HD3	2:B:161:GLU:OE2	2.19	0.41
1:A:50:LEU:HD11	5:A:2022:HOH:O	2.18	0.41
2:D:24:SER:HB2	2:D:30:VAL:HG11	2.01	0.41
1:C:9:CYS:O	1:C:224:ALA:HB2	2.20	0.41
2:F:97:ALA:HA	2:F:98:PRO:HD2	1.81	0.41
1:E:153:LEU:HD12	1:E:157:VAL:HG23	2.01	0.41
1:E:63:LEU:HD21	1:E:91:GLU:HG3	2.02	0.41
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.89	0.41
1:E:252:GLY:O	1:E:253:LEU:HG	2.20	0.41
1:A:169:LEU:HA	1:A:199:ILE:HB	2.02	0.41
1:E:143:TYR:O	1:E:146:LYS:HD2	2.21	0.41
1:E:123:GLN:NE2	1:E:123:GLN:H	2.05	0.41
1:E:127:VAL:HG21	1:E:160:VAL:HG13	2.02	0.41
1:A:53:THR:C	1:A:54:ALA:O	2.57	0.41
2:B:84:CYS:CB	2:B:178:HIS:CE1	3.04	0.41
2:D:189:LEU:O	2:D:189:LEU:HD13	2.21	0.41
1:A:140:VAL:O	1:A:149:THR:OG1	2.28	0.41
1:A:182:TYR:CZ	1:A:204:ALA:HB2	2.56	0.41
2:B:129:LYS:O	2:B:130:ASP:HB3	2.20	0.41
2:B:67:ILE:O	2:B:71:ARG:HB2	2.21	0.40
2:D:144:ARG:NH2	2:D:146:VAL:HG22	2.35	0.40
1:A:152:LEU:HD12	1:A:154:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:ILE:HD11	2:D:20:VAL:HG21	2.03	0.40
2:D:3:ILE:HD12	2:D:32:ILE:HD13	2.03	0.40
2:B:5:ILE:CD1	2:B:17:TYR:HA	2.51	0.40
1:E:195:THR:O	2:F:117:ARG:HG2	2.21	0.40
1:E:154:ARG:N	1:E:154:ARG:NH1	2.66	0.40
2:B:185:ILE:HA	2:B:188:LYS:HE3	2.02	0.40
2:F:92:GLU:OE2	2:F:107:GLU:HA	2.21	0.40
2:B:15:ASN:OD1	2:B:18:ARG:NH1	2.55	0.40
1:A:116:ILE:HB	1:A:125:VAL:HG22	2.04	0.40
2:D:97:ALA:HA	2:D:98:PRO:HD2	1.92	0.40
2:D:77:GLU:O	2:D:200:ARG:HD2	2.21	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	238/253 (94%)	222 (93%)	13 (6%)	3 (1%)	15	20
1	C	240/253 (95%)	226 (94%)	12 (5%)	2 (1%)	24	33
1	E	240/253 (95%)	217 (90%)	19 (8%)	4 (2%)	11	14
2	B	199/201 (99%)	182 (92%)	15 (8%)	2 (1%)	19	27
2	D	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	19	27
2	F	199/201 (99%)	176 (88%)	19 (10%)	4 (2%)	9	10
All	All	1315/1362 (96%)	1203 (92%)	95 (7%)	17 (1%)	15	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ALA

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Mol	Chain	Res	Type
1	A	251	GLU
1	C	251	GLU
1	E	54	ALA
1	E	251	GLU
1	C	225	SER
2	F	200	ARG
1	A	226	VAL
2	D	29	ASP
1	E	138	PHE
1	E	176	ASP
2	B	120	HIS
2	B	130	ASP
2	F	131	THR
2	F	130	ASP
2	D	98	PRO
2	F	51	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	198/208 (95%)	183 (92%)	15 (8%)	16 25
1	C	199/208 (96%)	183 (92%)	16 (8%)	15 22
1	E	200/208 (96%)	172 (86%)	28 (14%)	4 5
2	B	176/177 (99%)	157 (89%)	19 (11%)	8 10
2	D	176/177 (99%)	152 (86%)	24 (14%)	5 5
2	F	176/177 (99%)	150 (85%)	26 (15%)	4 4
All	All	1125/1155 (97%)	997 (89%)	128 (11%)	7 9

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	18	VAL

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	60	LYS
1	A	64	GLU
1	A	95	ARG
1	A	101	SER
1	A	115	GLN
1	A	123	GLN
1	A	154	ARG
1	A	162	LYS
1	A	191	ARG
1	A	230	ARG
1	A	235	ARG
1	A	253	LEU
2	B	16	LEU
2	B	29	ASP
2	B	45	LEU
2	B	65	ASP
2	B	107	GLU
2	B	118	LEU
2	B	124	ASN
2	B	148	GLU
2	B	153	LEU
2	B	155	THR
2	B	159	ASP
2	B	180	GLU
2	B	185	ILE
2	B	187	ARG
2	B	190	LEU
2	B	192	LYS
2	B	197	SER
2	B	198	LEU
2	B	199	SER
1	C	10	LEU
1	C	44	ILE
1	C	50	LEU
1	C	58	LYS
1	C	60	LYS
1	C	67	GLU
1	C	73	ILE
1	C	91	GLU
1	C	125	VAL
1	C	133	ARG

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Mol	Chain	Res	Type
1	C	154	ARG
1	C	169	LEU
1	C	176	ASP
1	C	225	SER
1	C	235	ARG
1	C	253	LEU
2	D	1	MET
2	D	5	ILE
2	D	25	GLU
2	D	45	LEU
2	D	56	GLU
2	D	65	ASP
2	D	75	GLU
2	D	89	LEU
2	D	104	SER
2	D	114	ARG
2	D	116	ARG
2	D	118	LEU
2	D	141	HIS
2	D	149	GLU
2	D	153	LEU
2	D	155	THR
2	D	157	GLU
2	D	161	GLU
2	D	180	GLU
2	D	185	ILE
2	D	187	ARG
2	D	189	LEU
2	D	190	LEU
2	D	199	SER
1	E	5	ARG
1	E	19	LYS
1	E	29	SER
1	E	34	GLU
1	E	35	LEU
1	E	37	LYS
1	E	50	LEU
1	E	60	LYS
1	E	64	GLU
1	E	67	GLU
1	E	73	ILE
1	E	95	ARG

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Mol	Chain	Res	Type
1	E	101	SER
1	E	109	ASN
1	E	118	GLN
1	E	123	GLN
1	E	125	VAL
1	E	132	LYS
1	E	146	LYS
1	E	153	LEU
1	E	154	ARG
1	E	162	LYS
1	E	174	ASP
1	E	176	ASP
1	E	195	THR
1	E	225	SER
1	E	235	ARG
1	E	250	LEU
2	F	1	MET
2	F	21	LYS
2	F	36	GLU
2	F	41	ASP
2	F	45	LEU
2	F	53	HIS
2	F	56	GLU
2	F	62	ARG
2	F	71	ARG
2	F	72	LYS
2	F	89	LEU
2	F	92	GLU
2	F	94	SER
2	F	107	GLU
2	F	109	ASN
2	F	116	ARG
2	F	118	LEU
2	F	124	ASN
2	F	148	GLU
2	F	149	GLU
2	F	153	LEU
2	F	180	GLU
2	F	185	ILE
2	F	190	LEU
2	F	198	LEU
2	F	199	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	109	ASN
1	A	123	GLN
1	A	209	HIS
2	B	53	HIS
2	B	120	HIS
2	B	124	ASN
2	B	178	HIS
1	C	84	HIS
1	C	109	ASN
1	C	115	GLN
1	C	118	GLN
2	D	88	GLN
2	D	176	GLN
1	E	109	ASN
1	E	118	GLN
1	E	123	GLN
1	E	209	HIS
2	F	124	ASN
2	F	141	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	1202	-	5,5,5	0.68	0	5,5,5	0.43	0
4	GOL	B	1201	-	5,5,5	0.30	0	5,5,5	0.47	0
4	GOL	B	1202	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GLN	B	1205	-	6,9,9	0.44	0	5,11,11	0.47	0
4	GOL	C	1254	-	5,5,5	0.41	0	5,5,5	0.35	0
4	GOL	D	1201	-	5,5,5	0.48	0	5,5,5	0.40	0
3	GLN	D	1205	-	6,9,9	0.40	0	5,11,11	0.81	0
4	GOL	E	1254	-	5,5,5	0.30	0	5,5,5	0.26	0
4	GOL	E	1255	-	5,5,5	0.27	0	5,5,5	0.54	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
4	GOL	A	1202	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1201	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1202	-	-	0/4/4/4	0/0/0/0
3	GLN	B	1205	-	-	0/5/9/9	0/0/0/0
4	GOL	C	1254	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1201	-	-	0/4/4/4	0/0/0/0
3	GLN	D	1205	-	-	0/5/9/9	0/0/0/0
4	GOL	E	1254	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1255	-	-	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1202	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1205	GLN	1	0
4	C	1254	GOL	2	0
4	E	1254	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, 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	242/253 (95%)	-0.38	2 (0%) 87 87	26, 41, 58, 77	0
1	C	244/253 (96%)	-0.35	3 (1%) 81 81	29, 41, 61, 73	0
1	E	244/253 (96%)	-0.14	4 (1%) 74 74	34, 50, 64, 74	0
2	B	201/201 (100%)	-0.48	0 100 100	28, 37, 52, 68	0
2	D	201/201 (100%)	-0.42	0 100 100	26, 37, 53, 73	0
2	F	201/201 (100%)	-0.30	3 (1%) 76 75	34, 46, 62, 72	0
All	All	1333/1362 (97%)	-0.34	12 (0%) 85 85	26, 43, 60, 77	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	5.5
1	E	253	LEU	4.0
2	F	201	ARG	3.2
1	E	251	GLU	2.8
1	C	253	LEU	2.7
2	F	199	SER	2.6
1	C	252	GLY	2.3
2	F	40	ASN	2.2
1	A	229	PHE	2.2
1	E	57	GLU	2.2
1	C	177	GLY	2.1
1	E	53	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	E	1255	6/6	0.92	0.15	0.93	44,45,46,47	0
3	GLN	D	1205	10/10	0.94	0.14	0.56	35,36,38,42	0
3	GLN	B	1205	10/10	0.95	0.12	0.22	27,28,30,31	0
4	GOL	D	1201	6/6	0.96	0.14	-	37,40,41,41	0
4	GOL	E	1254	6/6	0.96	0.07	-	42,42,42,43	0
4	GOL	B	1201	6/6	0.91	0.19	-	44,45,46,46	0
4	GOL	A	1202	6/6	0.93	0.12	-	38,39,40,41	0
4	GOL	C	1254	6/6	0.94	0.13	-	33,38,40,41	0
4	GOL	B	1202	6/6	0.93	0.11	-	44,48,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.