Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:59 AM GMT

PDB ID	:	2JLA
Title	:	CRYSTAL STRUCTURE OF E.COLI MEND, 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXADIENE-1-CARBOXYLATE SYNTHASE - SEMET PROTEIN
Authors	:	Dawson, A.; Fyfe, P.K.; Hunter, W.N.
Deposited on	:	2008-09-05
Resolution	:	2.81 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:

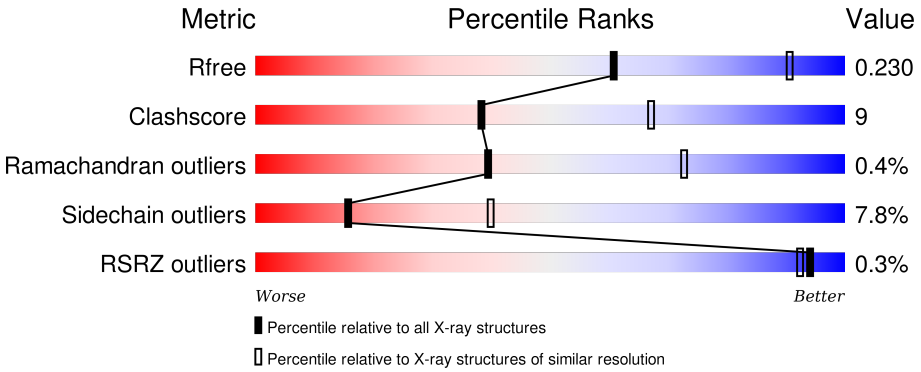
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	558	% 78% 19% •
1	B	558	79% 18% •
1	C	558	77% 19% •
1	D	558	77% 20% •

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
4	CL	D	1560	-	-	X	-

2 Entry composition

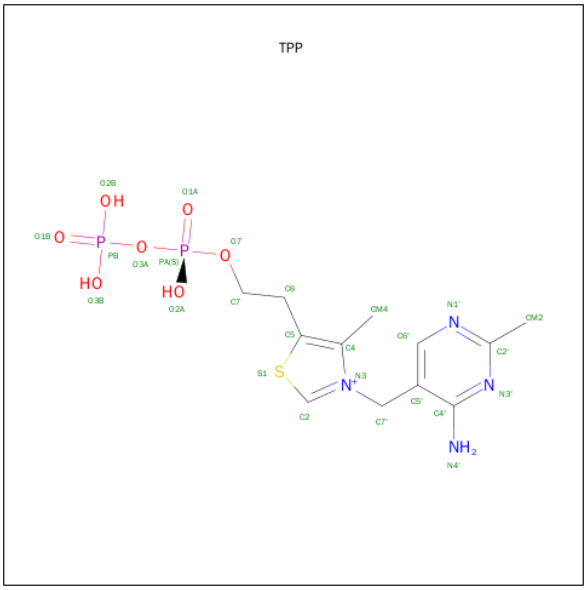
There are 5 unique types of molecules in this entry. The entry contains 17841 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	Se	0	0	0
			4331	2746	781	789	7	8			
1	B	556	Total	C	N	O	S	Se	0	0	0
			4331	2746	781	789	7	8			
1	C	556	Total	C	N	O	S	Se	0	0	0
			4331	2746	781	789	7	8			
1	D	556	Total	C	N	O	S	Se	0	0	0
			4331	2746	781	789	7	8			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	2	Total	Mn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cl	0	0
			4	4		
4	A	3	Total	Cl	0	0
			3	3		
4	D	3	Total	Cl	0	0
			3	3		
4	C	3	Total	Cl	0	0
			3	3		

- Molecule 5 is water.

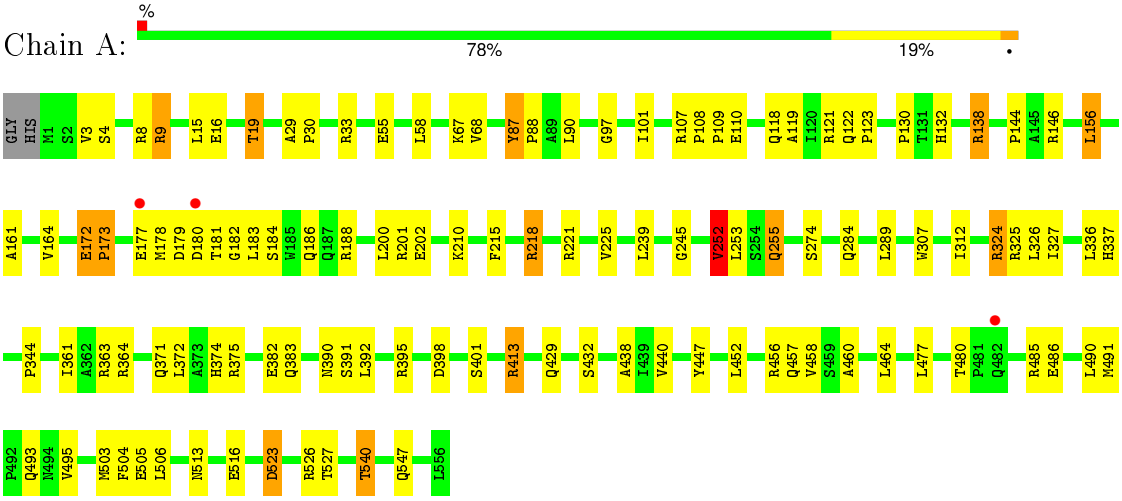
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	99	Total	O	0	0
			99	99		
5	C	87	Total	O	0	0
			87	87		
5	D	111	Total	O	0	0
			111	111		

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.

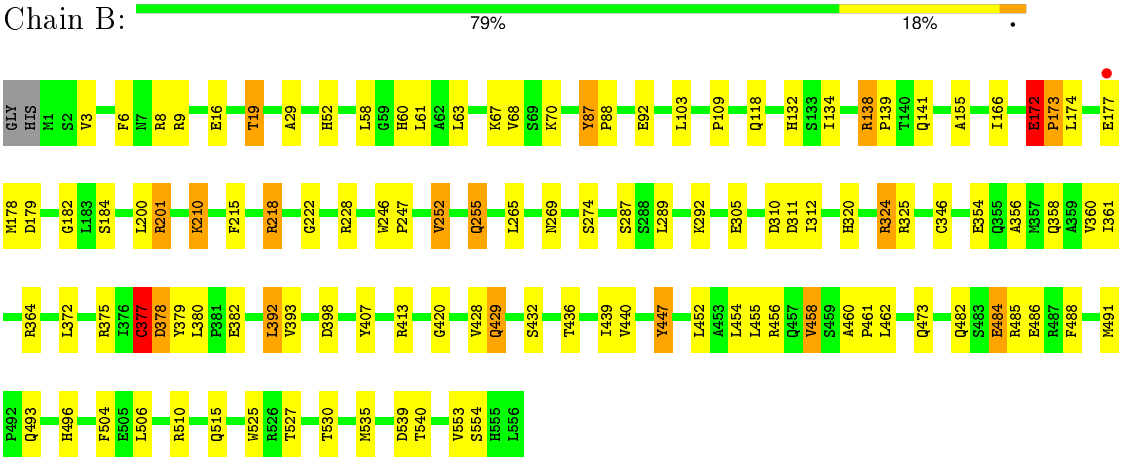
• Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

Chain A:



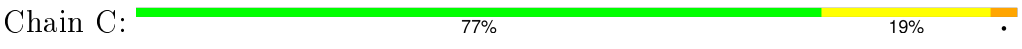
• Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

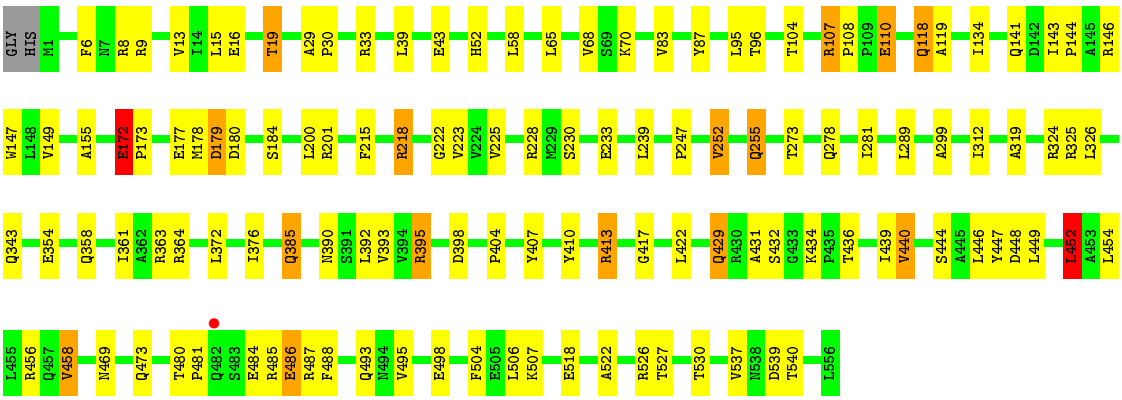
Chain B:



• Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

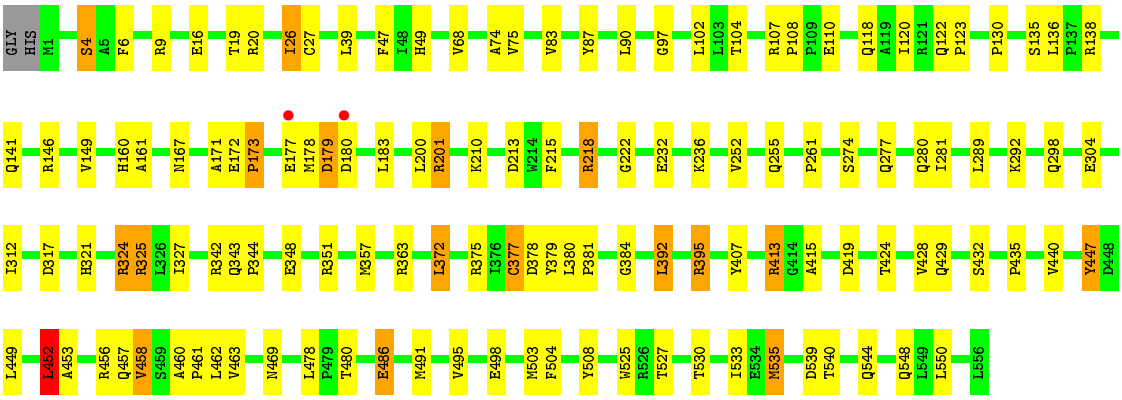
Chain C:





• Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	95.83Å 95.83Å 463.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.05 – 2.81 47.92 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.5 (83.05-2.81) 99.5 (47.92-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.169 , 0.233 0.170 , 0.230	Depositor DCC
R_{free} test set	2936 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.8	EDS
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 57816 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17841	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: CL, MN, TPP

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	0.48	0/4432	0.64	2/6033 (0.0%)
1	B	0.51	1/4432 (0.0%)	0.63	0/6033
1	C	0.52	1/4432 (0.0%)	0.65	2/6033 (0.0%)
1	D	0.51	2/4432 (0.0%)	0.64	2/6033 (0.0%)
All	All	0.50	4/17728 (0.0%)	0.64	6/24132 (0.0%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	486	GLU	CG-CD	-7.40	1.40	1.51
1	C	486	GLU	CG-CD	-7.39	1.40	1.51
1	D	486	GLU	CB-CG	-5.22	1.42	1.52
1	B	377	CYS	CB-SG	-5.12	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	452	LEU	CA-CB-CG	9.20	136.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	452	LEU	CA-CB-CG	9.17	136.40	115.30
1	A	172	GLU	C-N-CD	-6.84	105.55	120.60
1	A	252	VAL	CB-CA-C	-5.82	100.34	111.40
1	C	200	LEU	CA-CB-CG	5.71	128.42	115.30
1	D	173	PRO	N-CA-C	-5.45	97.93	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	GLU	Peptide
1	B	172	GLU	Peptide
1	C	172	GLU	Peptide
1	D	172	GLU	Peptide

5.2 Too-close contacts (i)

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	4331	0	4298	78	0
1	B	4331	0	4298	81	0
1	C	4331	0	4298	81	0
1	D	4331	0	4298	90	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	2	0
2	D	26	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	2	0
4	B	4	0	0	1	0
4	C	3	0	0	1	0
4	D	3	0	0	2	0
5	A	98	0	0	7	0
5	B	99	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	87	0	0	5	0
5	D	111	0	0	8	0
All	All	17841	0	17256	312	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 9.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:HG3	1:B:201:ARG:HH21	1.21	1.02
1:D:160:HIS:HB2	5:D:2035:HOH:O	1.64	0.97
1:D:16:GLU:O	1:D:19:THR:HB	1.64	0.97
1:A:395:ARG:HD3	5:A:2075:HOH:O	1.69	0.93
1:C:395:ARG:HD3	5:C:2058:HOH:O	1.70	0.91
1:A:523:ASP:HA	1:A:526:ARG:HH21	1.37	0.89
1:A:458:VAL:CG1	1:A:460:ALA:O	2.23	0.86
1:A:30:PRO:HG3	1:B:491:MSE:SE	2.28	0.84
1:C:172:GLU:HG2	1:C:172:GLU:O	1.78	0.83
1:A:371:GLN:O	1:A:375:ARG:HG2	1.76	0.83
1:C:312:ILE:O	1:C:325:ARG:NH2	2.15	0.79
1:A:458:VAL:HG12	1:A:460:ALA:O	1.82	0.79
1:B:8:ARG:HD3	1:B:178:MSE:HE1	1.64	0.78
1:D:312:ILE:O	1:D:325:ARG:NH2	2.16	0.78
1:B:172:GLU:O	1:B:172:GLU:HG2	1.83	0.77
1:C:252:VAL:CG2	1:C:398:ASP:HB2	2.15	0.76
1:C:413:ARG:NH2	4:C:1561:CL:CL	2.57	0.74
1:A:523:ASP:HA	1:A:526:ARG:NH2	2.02	0.74
1:C:449:LEU:O	1:C:452:LEU:CD2	2.37	0.72
1:C:252:VAL:HG22	1:C:398:ASP:HB2	1.72	0.72
1:B:496:HIS:NE2	5:B:2093:HOH:O	2.23	0.72
1:A:202:GLU:HG3	1:D:325:ARG:HB3	1.69	0.72
1:B:458:VAL:HG13	1:B:460:ALA:O	1.89	0.72
1:C:230:SER:OG	1:C:233:GLU:HG3	1.90	0.72
1:C:361:ILE:O	1:C:364:ARG:HG2	1.90	0.72
1:B:201:ARG:HG3	1:B:201:ARG:NH2	1.99	0.71
1:A:361:ILE:O	1:A:364:ARG:HG2	1.91	0.71
1:C:278:GLN:HG2	5:C:2040:HOH:O	1.91	0.71
1:C:108:PRO:HB2	1:C:110:GLU:OE2	1.90	0.71
1:A:109:PRO:HD2	1:A:138:ARG:HG3	1.73	0.70
1:B:361:ILE:O	1:B:364:ARG:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:HH21	1:C:180:ASP:HA	1.57	0.69
1:B:312:ILE:O	1:B:325:ARG:NH2	2.26	0.69
1:B:215:PHE:HA	1:B:218:ARG:HD2	1.75	0.68
1:A:456:ARG:NH2	1:B:493:GLN:O	2.27	0.67
1:A:16:GLU:O	1:A:19:THR:HB	1.95	0.67
1:D:458:VAL:HG13	1:D:460:ALA:O	1.94	0.67
1:D:413:ARG:NH2	4:D:1560:CL:CL	2.66	0.66
1:B:287:SER:HB2	5:B:2055:HOH:O	1.96	0.66
1:D:178:MSE:HE2	5:D:2039:HOH:O	1.96	0.66
1:A:108:PRO:HB2	1:A:110:GLU:OE2	1.96	0.66
1:A:107:ARG:HG3	1:A:119:ALA:HB2	1.78	0.65
1:A:9:ARG:HH12	1:A:180:ASP:HA	1.61	0.65
1:C:506:LEU:HD22	1:C:530:THR:HB	1.79	0.65
1:D:449:LEU:O	1:D:452:LEU:CD2	2.44	0.65
1:D:9:ARG:HH21	1:D:180:ASP:HA	1.62	0.65
1:A:413:ARG:HH11	1:A:413:ARG:CG	2.10	0.64
1:D:449:LEU:O	1:D:452:LEU:HD22	1.97	0.64
1:C:215:PHE:HA	1:C:218:ARG:HD2	1.79	0.63
1:B:393:VAL:HG21	1:B:439:ILE:HG12	1.80	0.63
1:A:413:ARG:HG3	1:A:413:ARG:NH1	2.12	0.63
1:B:392:LEU:HB2	2:B:1557:TPP:O1B	1.98	0.63
1:C:480:THR:OG1	1:C:485:ARG:HD3	1.98	0.63
1:B:540:THR:HG23	5:B:2098:HOH:O	1.99	0.62
1:D:210:LYS:HD3	5:D:2045:HOH:O	1.98	0.62
1:C:39:LEU:O	1:C:43:GLU:HG2	2.00	0.61
1:A:29:ALA:HB2	1:A:58:LEU:HD22	1.82	0.61
1:C:449:LEU:O	1:C:452:LEU:HD23	2.00	0.61
1:A:312:ILE:O	1:A:325:ARG:NH2	2.34	0.60
1:A:540:THR:HG23	5:A:2095:HOH:O	2.01	0.59
1:B:458:VAL:CG1	1:B:460:ALA:O	2.50	0.59
1:A:215:PHE:HA	1:A:218:ARG:HD2	1.82	0.59
1:A:505:GLU:OE1	4:A:1561:CL:CL	2.59	0.58
1:A:392:LEU:HB2	2:A:1557:TPP:O1B	2.02	0.58
1:B:16:GLU:O	1:B:19:THR:HB	2.03	0.58
1:C:493:GLN:O	1:D:456:ARG:NH2	2.37	0.58
1:D:19:THR:HG22	1:D:20:ARG:HD3	1.86	0.57
1:C:146:ARG:HA	1:C:149:VAL:HG12	1.85	0.57
1:A:8:ARG:HD3	1:A:178:MSE:HE1	1.86	0.57
1:D:83:VAL:HG13	1:D:104:THR:HG21	1.85	0.57
1:A:245:GLY:O	1:A:344:PRO:HA	2.05	0.57
1:C:252:VAL:HG22	1:C:398:ASP:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:VAL:HG21	1:C:439:ILE:HG12	1.87	0.57
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.87	0.57
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.40	0.57
1:B:52:HIS:HB2	1:B:454:LEU:HD21	1.86	0.56
1:C:16:GLU:O	1:C:19:THR:HB	2.05	0.56
1:A:221:ARG:HD3	5:A:2038:HOH:O	2.04	0.56
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.69	0.56
1:D:372:LEU:HD12	1:D:535:MSE:HE2	1.86	0.56
1:D:26:ILE:CD1	1:D:49:HIS:CD2	2.88	0.56
1:D:26:ILE:HD11	1:D:47:PHE:HB3	1.86	0.56
1:A:493:GLN:O	1:B:456:ARG:NH2	2.37	0.55
1:C:449:LEU:O	1:C:452:LEU:HD22	2.07	0.55
1:D:107:ARG:NH2	1:D:118:GLN:HB3	2.22	0.54
1:C:392:LEU:HB2	2:C:1557:TPP:O1B	2.07	0.54
1:D:457:GLN:HB2	5:D:2094:HOH:O	2.07	0.54
1:B:358:GLN:HG3	5:B:2067:HOH:O	2.06	0.54
1:A:486:GLU:HA	1:A:490:LEU:HD12	1.90	0.54
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.90	0.54
1:B:172:GLU:HB2	1:B:174:LEU:HG	1.87	0.54
1:D:424:THR:O	1:D:428:VAL:HG23	2.08	0.54
1:C:52:HIS:HB2	1:C:454:LEU:HD21	1.90	0.53
1:A:67:LYS:HD3	5:A:2080:HOH:O	2.08	0.53
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.43	0.53
1:A:523:ASP:CA	1:A:526:ARG:NH2	2.72	0.53
1:D:392:LEU:HB2	2:D:1557:TPP:O1B	2.09	0.53
1:D:381:PRO:HG2	1:D:384:GLY:HA3	1.90	0.53
1:C:65:LEU:HA	1:C:431:ALA:HB2	1.91	0.53
1:A:110:GLU:HG3	1:C:143:ILE:HG12	1.90	0.52
1:B:484:GLU:HB2	1:B:488:PHE:HD1	1.74	0.52
1:B:201:ARG:HE	1:C:324:ARG:NH1	2.08	0.52
1:C:118:GLN:HB3	1:D:415:ALA:O	2.09	0.52
1:C:107:ARG:HG3	1:C:119:ALA:HB2	1.90	0.52
1:C:52:HIS:C	1:D:491:MSE:HE1	2.30	0.52
1:B:132:HIS:HB3	5:B:2023:HOH:O	2.08	0.52
1:C:96:THR:HG22	1:C:228:ARG:NH2	2.24	0.52
1:A:252:VAL:HG22	1:A:398:ASP:HB2	1.91	0.52
1:A:413:ARG:CG	1:A:413:ARG:NH1	2.69	0.52
1:C:134:ILE:HD11	1:C:155:ALA:HB2	1.92	0.52
1:C:30:PRO:HG3	1:D:491:MSE:SE	2.59	0.52
1:B:305:GLU:OE2	1:B:324:ARG:NH1	2.44	0.51
1:C:9:ARG:NH2	1:C:180:ASP:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:HG2	5:A:2073:HOH:O	2.10	0.51
1:B:118:GLN:O	1:B:118:GLN:HG2	2.10	0.51
1:D:461:PRO:HB2	1:D:525:TRP:HE3	1.73	0.51
1:A:374:HIS:O	1:A:401:SER:HB3	2.11	0.51
1:A:144:PRO:HB2	1:A:146:ARG:HG2	1.93	0.51
1:A:523:ASP:HB3	1:A:526:ARG:HH22	1.76	0.51
1:D:540:THR:HG23	1:D:544:GLN:OE1	2.11	0.51
1:B:134:ILE:HD11	1:B:155:ALA:HB2	1.92	0.51
1:B:473:GLN:HG3	1:B:539:ASP:O	2.11	0.51
1:A:225:VAL:O	1:A:284:GLN:HA	2.11	0.51
1:B:269:ASN:HD22	1:B:554:SER:HA	1.75	0.50
1:C:222:GLY:HA2	1:C:281:ILE:O	2.12	0.50
1:D:90:LEU:HD21	1:D:130:PRO:HG3	1.94	0.50
1:D:26:ILE:HD11	1:D:49:HIS:CD2	2.46	0.50
1:A:9:ARG:HD3	1:A:181:THR:O	2.11	0.49
1:D:453:ALA:O	1:D:456:ARG:HD3	2.12	0.49
1:D:68:VAL:CG2	1:D:428:VAL:HG13	2.42	0.49
1:C:498:GLU:HB3	5:C:2070:HOH:O	2.12	0.49
1:A:8:ARG:HD3	1:A:178:MSE:CE	2.42	0.49
1:A:132:HIS:HB2	1:A:164:VAL:HG13	1.94	0.49
1:C:390:ASN:ND2	1:C:417:GLY:O	2.45	0.49
1:A:19:THR:HG21	5:A:2004:HOH:O	2.12	0.49
1:D:413:ARG:HG2	5:D:2062:HOH:O	2.13	0.49
1:B:61:LEU:HD13	1:B:454:LEU:HD13	1.94	0.49
1:B:456:ARG:HD2	1:B:504:PHE:HB3	1.95	0.49
1:D:363:ARG:NH2	1:D:548:GLN:OE1	2.46	0.49
1:A:68:VAL:HG11	1:A:432:SER:HB3	1.93	0.49
1:D:363:ARG:HD2	5:D:2076:HOH:O	2.13	0.49
1:B:482:GLN:HA	1:B:485:ARG:HH21	1.77	0.48
1:D:90:LEU:HD13	1:D:102:LEU:HD11	1.94	0.48
1:A:327:ILE:HD12	1:A:327:ILE:N	2.29	0.48
1:B:310:ASP:OD1	1:B:311:ASP:N	2.47	0.48
1:D:4:SER:HB3	5:D:2002:HOH:O	2.13	0.48
1:B:138:ARG:NH1	5:B:2026:HOH:O	2.47	0.48
1:D:498:GLU:HB2	1:D:508:TYR:CE2	2.48	0.48
1:B:429:GLN:HB2	1:B:436:THR:OG1	2.13	0.48
1:A:55:GLU:OE1	1:B:447:TYR:OH	2.21	0.48
1:A:110:GLU:OE2	1:A:138:ARG:HD2	2.14	0.48
1:D:463:VAL:HG13	1:D:533:ILE:HD12	1.95	0.48
1:C:225:VAL:HG11	1:C:289:LEU:HD21	1.94	0.48
1:D:456:ARG:HD2	1:D:504:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:PHE:HA	1:D:218:ARG:HD2	1.96	0.48
1:D:343:GLN:NE2	1:D:344:PRO:HD2	2.29	0.48
1:D:539:ASP:OD1	1:D:540:THR:N	2.46	0.47
1:C:469:ASN:HB2	1:C:539:ASP:HA	1.96	0.47
1:A:87:TYR:HB3	1:A:88:PRO:HD3	1.96	0.47
1:B:222:GLY:HA3	1:B:246:TRP:CD2	2.49	0.47
1:B:172:GLU:O	1:B:172:GLU:CG	2.60	0.47
1:B:255:GLN:HG2	1:B:407:TYR:O	2.14	0.47
1:B:68:VAL:HG11	1:B:432:SER:HB3	1.96	0.47
1:D:461:PRO:HB2	1:D:525:TRP:CE3	2.49	0.47
1:B:9:ARG:HD2	1:B:182:GLY:C	2.34	0.47
1:B:484:GLU:HA	5:B:2090:HOH:O	2.13	0.47
1:A:390:ASN:HB3	4:A:1560:CL:CL	2.52	0.47
1:C:179:ASP:OD1	1:C:179:ASP:C	2.52	0.47
1:D:136:LEU:HB2	1:D:167:ASN:O	2.15	0.47
1:D:463:VAL:CG1	1:D:533:ILE:HD12	2.45	0.47
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.50	0.47
1:D:395:ARG:NH2	4:D:1560:CL:CL	2.83	0.47
1:A:90:LEU:HD21	1:A:130:PRO:HG3	1.97	0.47
1:A:9:ARG:HG3	1:A:186:GLN:CD	2.36	0.47
1:D:26:ILE:HD12	1:D:49:HIS:CD2	2.50	0.47
1:A:456:ARG:HG3	1:A:506:LEU:HD21	1.97	0.46
1:A:4:SER:HB2	5:A:2030:HOH:O	2.14	0.46
1:B:228:ARG:HG3	5:B:2085:HOH:O	2.16	0.46
1:D:280:GLN:O	1:D:304:GLU:HB3	2.15	0.46
1:D:68:VAL:HG21	1:D:428:VAL:HG13	1.96	0.46
1:B:356:ALA:O	1:B:360:VAL:HG23	2.15	0.46
1:A:110:GLU:CG	1:C:143:ILE:HG12	2.46	0.46
1:B:461:PRO:HB2	1:B:525:TRP:HE3	1.81	0.46
1:A:122:GLN:N	1:A:123:PRO:CD	2.79	0.46
1:A:253:LEU:HD11	1:A:413:ARG:HG2	1.98	0.46
1:B:201:ARG:NE	1:C:324:ARG:HH11	2.13	0.46
1:C:413:ARG:CG	1:C:413:ARG:HH11	2.29	0.46
1:B:377:CYS:HA	1:B:380:LEU:HG	1.98	0.46
1:B:452:LEU:HD23	1:B:455:LEU:HD12	1.97	0.45
1:D:232:GLU:O	1:D:236:LYS:HD2	2.16	0.45
1:C:446:LEU:HD21	1:D:503:MSE:HE2	1.98	0.45
1:D:118:GLN:O	1:D:118:GLN:HG2	2.17	0.45
1:C:456:ARG:HD2	1:C:504:PHE:HB3	1.97	0.45
1:A:513:ASN:OD1	1:A:516:GLU:HG3	2.16	0.45
1:C:299:ALA:HA	1:C:319:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLN:CG	1:B:458:VAL:HG22	2.46	0.45
1:B:265:LEU:HB3	1:B:553:VAL:HG21	1.98	0.45
1:A:118:GLN:HG2	1:A:118:GLN:O	2.17	0.45
1:B:103:LEU:HD23	1:B:166:ILE:HB	1.98	0.45
1:B:375:ARG:O	1:B:378:ASP:HB2	2.16	0.45
1:A:456:ARG:HD2	1:A:504:PHE:HB3	1.98	0.45
1:C:540:THR:HG23	5:C:2080:HOH:O	2.17	0.45
1:B:68:VAL:HG21	1:B:428:VAL:HG13	1.99	0.45
1:B:210:LYS:HD3	5:B:2046:HOH:O	2.15	0.45
1:C:325:ARG:NH1	1:C:326:LEU:O	2.50	0.45
1:B:429:GLN:HG2	1:B:458:VAL:HG22	1.99	0.45
1:B:109:PRO:HD2	1:B:138:ARG:HG3	1.97	0.45
1:C:473:GLN:HG3	1:C:539:ASP:O	2.17	0.45
1:B:68:VAL:CG2	1:B:428:VAL:HG13	2.47	0.45
1:B:462:LEU:O	1:B:530:THR:HA	2.16	0.45
1:C:223:VAL:HG22	1:C:247:PRO:HG2	1.99	0.45
1:D:26:ILE:HG23	1:D:74:ALA:HB3	1.98	0.45
1:D:469:ASN:HB2	1:D:539:ASP:HA	1.98	0.45
1:B:252:VAL:HG13	1:B:398:ASP:HA	1.98	0.45
1:D:380:LEU:HB3	1:D:407:TYR:CZ	2.52	0.44
1:C:434:LYS:HE2	5:C:2056:HOH:O	2.17	0.44
1:B:364:ARG:O	1:B:375:ARG:NH2	2.50	0.44
1:B:252:VAL:HG22	1:B:398:ASP:HB2	1.99	0.44
1:C:422:LEU:HD12	1:C:448:ASP:O	2.17	0.44
1:C:134:ILE:HD11	1:C:155:ALA:CB	2.47	0.44
1:B:530:THR:O	4:B:1562:CL:CL	2.72	0.44
1:D:419:ASP:HB3	1:D:447:TYR:CZ	2.53	0.44
1:D:261:PRO:HB2	1:D:357:MSE:HE2	2.00	0.44
1:A:336:LEU:HD23	1:A:337:HIS:CE1	2.52	0.44
2:C:1557:TPP:C2	2:C:1557:TPP:HN42	2.30	0.44
1:B:29:ALA:HB2	1:B:58:LEU:HD22	1.99	0.44
1:C:507:LYS:HB2	1:C:507:LYS:HE3	1.81	0.44
1:A:9:ARG:HG3	1:A:186:GLN:NE2	2.33	0.44
1:A:101:ILE:HD11	1:A:156:LEU:HD21	1.99	0.44
1:C:343:GLN:HA	1:C:343:GLN:OE1	2.17	0.44
1:D:377:CYS:C	1:D:379:TYR:H	2.21	0.44
1:D:277:GLN:NE2	5:D:2059:HOH:O	2.51	0.44
1:C:8:ARG:HD3	1:C:178:MSE:HE1	2.00	0.44
1:B:491:MSE:HE2	1:B:491:MSE:HB3	1.92	0.43
1:D:108:PRO:HG3	1:D:171:ALA:HA	2.00	0.43
1:B:311:ASP:HB2	5:B:2061:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HG2	1:A:182:GLY:O	2.17	0.43
1:D:419:ASP:HB3	1:D:447:TYR:CE2	2.53	0.43
1:B:3:VAL:HB	1:B:173:PRO:HD2	2.00	0.43
1:D:478:LEU:O	1:D:480:THR:N	2.48	0.43
1:C:429:GLN:HG2	1:C:458:VAL:CG2	2.49	0.43
1:A:491:MSE:HB3	1:A:491:MSE:HE2	1.81	0.43
1:C:452:LEU:HB2	1:C:506:LEU:HD11	2.01	0.43
1:D:27:CYS:HB2	1:D:75:VAL:HG22	2.00	0.43
1:D:146:ARG:HA	1:D:149:VAL:HG12	2.01	0.43
1:C:404:PRO:HG2	1:C:407:TYR:HB2	2.00	0.43
1:B:63:LEU:HD21	1:B:92:GLU:HG2	2.01	0.42
1:A:480:THR:OG1	1:A:485:ARG:HD3	2.19	0.42
1:C:539:ASP:OD1	1:C:540:THR:N	2.52	0.42
1:B:70:LYS:HA	1:B:70:LYS:HD2	1.83	0.42
1:D:107:ARG:HH21	1:D:118:GLN:HB3	1.83	0.42
1:A:3:VAL:HB	1:A:173:PRO:HD2	2.01	0.42
1:D:222:GLY:HA2	1:D:281:ILE:O	2.19	0.42
1:B:247:PRO:HG3	1:B:346:CYS:SG	2.60	0.42
1:D:298:GLN:O	1:D:321:HIS:HE1	2.01	0.42
1:A:255:GLN:HE21	1:A:255:GLN:HB2	1.64	0.42
1:B:320:HIS:CE1	1:C:147:TRP:HD1	2.38	0.42
1:B:60:HIS:CG	1:B:420:GLY:HA3	2.55	0.42
1:C:449:LEU:HD23	1:D:449:LEU:HD23	2.02	0.42
1:A:503:MSE:HE3	1:B:496:HIS:O	2.19	0.42
1:D:83:VAL:HG13	1:D:104:THR:CG2	2.50	0.42
1:B:506:LEU:HD22	1:B:530:THR:HB	2.02	0.42
1:A:477:LEU:HD12	1:A:547:GLN:HE21	1.85	0.41
1:D:179:ASP:OD1	1:D:179:ASP:C	2.57	0.41
1:A:438:ALA:O	1:A:464:LEU:HA	2.20	0.41
1:C:9:ARG:O	1:C:13:VAL:HG23	2.20	0.41
1:D:458:VAL:CG1	1:D:460:ALA:O	2.66	0.41
1:D:26:ILE:HD12	1:D:49:HIS:HD2	1.85	0.41
1:B:222:GLY:HA3	1:B:246:TRP:CE2	2.55	0.41
1:D:97:GLY:HA2	1:D:161:ALA:HB1	2.01	0.41
1:A:179:ASP:C	1:A:179:ASP:OD1	2.57	0.41
1:D:377:CYS:C	1:D:379:TYR:N	2.72	0.41
1:D:201:ARG:H	1:D:201:ARG:HG2	1.70	0.41
1:C:146:ARG:HE	1:C:146:ARG:HB3	1.76	0.41
1:D:122:GLN:N	1:D:123:PRO:CD	2.84	0.41
1:D:449:LEU:O	1:D:452:LEU:HD23	2.19	0.41
1:C:144:PRO:HB2	1:C:146:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:LEU:HD12	1:D:392:LEU:HA	1.97	0.41
1:D:462:LEU:HD22	1:D:530:THR:HG23	2.01	0.41
1:C:95:LEU:HD11	1:D:120:ILE:HG22	2.02	0.41
1:A:16:GLU:HA	1:A:16:GLU:OE1	2.21	0.41
1:C:29:ALA:HB2	1:C:58:LEU:HD22	2.02	0.41
1:C:481:PRO:HG3	1:D:39:LEU:HD11	2.02	0.41
1:A:122:GLN:H	1:A:123:PRO:HD3	1.86	0.41
1:A:110:GLU:CD	1:A:138:ARG:HH11	2.23	0.41
1:B:377:CYS:C	1:B:379:TYR:N	2.74	0.41
1:A:325:ARG:NH1	1:A:326:LEU:O	2.50	0.41
1:C:68:VAL:HG22	1:C:410:TYR:CZ	2.56	0.41
1:D:26:ILE:HD11	1:D:47:PHE:CB	2.49	0.41
1:B:255:GLN:HB2	1:B:255:GLN:HE21	1.71	0.41
1:C:429:GLN:CD	1:C:458:VAL:HG22	2.40	0.41
1:A:97:GLY:HA2	1:A:161:ALA:HB1	2.01	0.41
1:C:522:ALA:O	1:C:526:ARG:HG3	2.21	0.41
1:C:440:VAL:HG13	1:C:444:SER:HB2	2.03	0.41
1:D:213:ASP:OD1	1:D:324:ARG:NH1	2.53	0.41
1:A:477:LEU:HD12	1:A:547:GLN:NE2	2.35	0.41
1:C:385:GLN:NE2	1:C:436:THR:OG1	2.49	0.41
1:B:63:LEU:O	1:B:67:LYS:HB2	2.21	0.40
1:B:377:CYS:O	1:B:378:ASP:C	2.59	0.40
1:B:138:ARG:HA	1:B:139:PRO:HD3	1.93	0.40
1:C:487:ARG:HD3	1:C:488:PHE:CE1	2.56	0.40
1:D:381:PRO:HB2	1:D:435:PRO:HB2	2.03	0.40
1:D:108:PRO:HB2	1:D:110:GLU:OE2	2.20	0.40
1:C:255:GLN:HG2	1:C:407:TYR:O	2.21	0.40
1:C:376:ILE:HD12	1:C:376:ILE:HA	1.89	0.40
1:C:413:ARG:HG3	1:C:413:ARG:NH1	2.35	0.40
1:D:90:LEU:HD13	1:D:102:LEU:CD1	2.51	0.40
1:D:110:GLU:CD	1:D:110:GLU:H	2.25	0.40
1:D:317:ASP:OD2	1:D:321:HIS:HB2	2.21	0.40
1:C:83:VAL:HG13	1:C:104:THR:HG21	2.04	0.40
1:A:307:TRP:CD1	1:A:324:ARG:HG3	2.56	0.40
1:B:87:TYR:HB3	1:B:88:PRO:HD3	2.02	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	554/558 (99%)	526 (95%)	26 (5%)	2 (0%)	39	73
1	B	554/558 (99%)	529 (96%)	23 (4%)	2 (0%)	39	73
1	C	554/558 (99%)	524 (95%)	28 (5%)	2 (0%)	39	73
1	D	554/558 (99%)	531 (96%)	21 (4%)	2 (0%)	39	73
All	All	2216/2232 (99%)	2110 (95%)	98 (4%)	8 (0%)	39	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	PRO
1	D	173	PRO
1	B	378	ASP
1	C	118	GLN
1	C	173	PRO
1	D	378	ASP
1	A	391	SER
1	B	173	PRO

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	452/445 (102%)	417 (92%)	35 (8%)	16	40
1	B	452/445 (102%)	419 (93%)	33 (7%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	452/445 (102%)	417 (92%)	35 (8%)	16 40
1	D	452/445 (102%)	414 (92%)	38 (8%)	14 36
All	All	1808/1780 (102%)	1667 (92%)	141 (8%)	16 40

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	15	LEU
1	A	19	THR
1	A	33	ARG
1	A	87	TYR
1	A	121	ARG
1	A	138	ARG
1	A	156	LEU
1	A	177	GLU
1	A	183	LEU
1	A	184	SER
1	A	188	ARG
1	A	200	LEU
1	A	201	ARG
1	A	210	LYS
1	A	218	ARG
1	A	239	LEU
1	A	252	VAL
1	A	255	GLN
1	A	274	SER
1	A	289	LEU
1	A	324	ARG
1	A	363	ARG
1	A	372	LEU
1	A	382	GLU
1	A	413	ARG
1	A	429	GLN
1	A	440	VAL
1	A	447	TYR
1	A	452	LEU
1	A	457	GLN
1	A	495	VAL
1	A	523	ASP
1	A	527	THR

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Mol	Chain	Res	Type
1	A	540	THR
1	B	19	THR
1	B	87	TYR
1	B	138	ARG
1	B	172	GLU
1	B	177	GLU
1	B	179	ASP
1	B	184	SER
1	B	200	LEU
1	B	201	ARG
1	B	210	LYS
1	B	218	ARG
1	B	252	VAL
1	B	255	GLN
1	B	274	SER
1	B	289	LEU
1	B	292	LYS
1	B	324	ARG
1	B	354	GLU
1	B	372	LEU
1	B	377	CYS
1	B	382	GLU
1	B	392	LEU
1	B	413	ARG
1	B	429	GLN
1	B	440	VAL
1	B	447	TYR
1	B	458	VAL
1	B	484	GLU
1	B	486	GLU
1	B	510	ARG
1	B	515	GLN
1	B	527	THR
1	B	535	MSE
1	C	15	LEU
1	C	19	THR
1	C	33	ARG
1	C	70	LYS
1	C	87	TYR
1	C	107	ARG
1	C	110	GLU
1	C	172	GLU

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Mol	Chain	Res	Type
1	C	177	GLU
1	C	179	ASP
1	C	184	SER
1	C	201	ARG
1	C	218	ARG
1	C	239	LEU
1	C	252	VAL
1	C	255	GLN
1	C	273	THR
1	C	354	GLU
1	C	358	GLN
1	C	363	ARG
1	C	372	LEU
1	C	385	GLN
1	C	395	ARG
1	C	413	ARG
1	C	429	GLN
1	C	440	VAL
1	C	447	TYR
1	C	452	LEU
1	C	458	VAL
1	C	484	GLU
1	C	486	GLU
1	C	495	VAL
1	C	518	GLU
1	C	527	THR
1	C	537	VAL
1	D	4	SER
1	D	26	ILE
1	D	87	TYR
1	D	135	SER
1	D	138	ARG
1	D	177	GLU
1	D	179	ASP
1	D	183	LEU
1	D	200	LEU
1	D	201	ARG
1	D	218	ARG
1	D	252	VAL
1	D	255	GLN
1	D	274	SER
1	D	289	LEU

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Mol	Chain	Res	Type
1	D	292	LYS
1	D	324	ARG
1	D	325	ARG
1	D	327	ILE
1	D	342	ARG
1	D	348	GLU
1	D	351	ARG
1	D	372	LEU
1	D	375	ARG
1	D	377	CYS
1	D	392	LEU
1	D	395	ARG
1	D	413	ARG
1	D	429	GLN
1	D	440	VAL
1	D	447	TYR
1	D	452	LEU
1	D	458	VAL
1	D	486	GLU
1	D	495	VAL
1	D	527	THR
1	D	535	MSE
1	D	550	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	B	129	HIS
1	B	269	ASN
1	B	544	GLN
1	C	280	GLN
1	C	355	GLN
1	C	538	ASN
1	D	117	ASN
1	D	296	GLN
1	D	343	GLN
1	D	355	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 18 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	TPP	A	1557	3	20,27,27	1.55	3 (15%)	31,40,40	1.82	6 (19%)
2	TPP	B	1557	3	20,27,27	1.53	5 (25%)	31,40,40	1.89	9 (29%)
2	TPP	C	1557	3	20,27,27	1.61	4 (20%)	31,40,40	1.83	9 (29%)
2	TPP	D	1557	3	20,27,27	1.49	4 (20%)	31,40,40	1.89	11 (35%)

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
2	TPP	A	1557	3	-	0/16/17/17	0/2/2/2
2	TPP	B	1557	3	-	0/16/17/17	0/2/2/2
2	TPP	C	1557	3	-	0/16/17/17	0/2/2/2
2	TPP	D	1557	3	-	0/16/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1557	TPP	C4-N3	-3.46	1.36	1.39
2	A	1557	TPP	C4-N3	-3.25	1.36	1.39
2	B	1557	TPP	C4-N3	-2.46	1.37	1.39
2	D	1557	TPP	PB-O2B	2.24	1.62	1.54
2	C	1557	TPP	PB-O2B	2.26	1.62	1.54
2	B	1557	TPP	PB-O2B	2.28	1.62	1.54
2	B	1557	TPP	CM4-C4	2.33	1.54	1.49
2	D	1557	TPP	CM4-C4	2.44	1.55	1.49
2	C	1557	TPP	PB-O1B	2.53	1.59	1.51
2	B	1557	TPP	PA-O1A	2.71	1.61	1.51
2	D	1557	TPP	PA-O1A	2.83	1.61	1.51
2	A	1557	TPP	PB-O1B	3.02	1.61	1.51
2	D	1557	TPP	PB-O1B	3.32	1.62	1.51
2	A	1557	TPP	PA-O1A	3.61	1.64	1.51
2	C	1557	TPP	PA-O1A	3.62	1.64	1.51
2	B	1557	TPP	PB-O1B	3.63	1.63	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1557	TPP	CM4-C4-C5	-3.69	120.60	128.90
2	B	1557	TPP	CM4-C4-C5	-3.65	120.69	128.90
2	A	1557	TPP	CM4-C4-C5	-3.34	121.39	128.90
2	C	1557	TPP	CM4-C4-C5	-3.33	121.42	128.90
2	B	1557	TPP	N1'-C2'-N3'	-2.94	120.17	125.60
2	A	1557	TPP	N1'-C2'-N3'	-2.74	120.52	125.60
2	D	1557	TPP	C7'-C5'-C6'	-2.74	115.06	120.67
2	D	1557	TPP	N1'-C2'-N3'	-2.64	120.72	125.60
2	C	1557	TPP	N1'-C2'-N3'	-2.38	121.19	125.60
2	B	1557	TPP	C5'-C6'-N1'	-2.37	119.74	123.86
2	C	1557	TPP	C5'-C6'-N1'	-2.27	119.93	123.86
2	D	1557	TPP	PA-O3A-PB	-2.12	125.57	132.67
2	C	1557	TPP	PA-O3A-PB	-2.11	125.59	132.67
2	D	1557	TPP	C5'-C6'-N1'	-2.11	120.20	123.86
2	B	1557	TPP	C7'-C5'-C6'	-2.02	116.53	120.67
2	D	1557	TPP	O3B-PB-O3A	2.09	114.58	105.09
2	C	1557	TPP	CM2-C2'-N1'	2.19	119.66	117.03
2	D	1557	TPP	C6-C5-C4	2.33	129.66	127.56
2	D	1557	TPP	C6-C5-S1	2.58	123.85	120.24
2	B	1557	TPP	CM2-C2'-N1'	2.63	120.18	117.03
2	B	1557	TPP	O3B-PB-O3A	2.78	117.69	105.09
2	C	1557	TPP	C6'-N1'-C2'	2.92	120.87	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1557	TPP	C6'-N1'-C2'	2.94	120.90	115.77
2	C	1557	TPP	O3B-PB-O3A	2.95	118.50	105.09
2	D	1557	TPP	C5-C4-N3	3.03	114.36	107.69
2	A	1557	TPP	C6'-N1'-C2'	3.08	121.16	115.77
2	A	1557	TPP	C5-C4-N3	3.12	114.55	107.69
2	A	1557	TPP	O3B-PB-O3A	3.17	119.47	105.09
2	C	1557	TPP	C5-C4-N3	3.23	114.80	107.69
2	B	1557	TPP	C5-C4-N3	3.24	114.81	107.69
2	D	1557	TPP	CM2-C2'-N1'	3.60	121.35	117.03
2	B	1557	TPP	C6'-N1'-C2'	3.71	122.25	115.77
2	B	1557	TPP	C6-C5-C4	4.04	131.19	127.56
2	C	1557	TPP	C6-C5-C4	4.19	131.32	127.56
2	A	1557	TPP	C6-C5-C4	4.55	131.64	127.56

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
2	A	1557	TPP	1	0
2	B	1557	TPP	1	0
2	C	1557	TPP	2	0
2	D	1557	TPP	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	548/558 (98%)	-0.49	3 (0%)	91	88	12, 18, 28, 37	6 (1%)
1	B	548/558 (98%)	-0.51	1 (0%)	95	94	12, 18, 29, 37	7 (1%)
1	C	548/558 (98%)	-0.51	1 (0%)	95	94	12, 18, 29, 37	5 (0%)
1	D	548/558 (98%)	-0.48	2 (0%)	93	90	12, 18, 29, 37	6 (1%)
All	All	2192/2232 (98%)	-0.50	7 (0%)	94	92	12, 18, 29, 37	24 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	3.1
1	A	482	GLN	2.7
1	D	180	ASP	2.6
1	D	177	GLU	2.4
1	C	482	GLN	2.3
1	B	177	GLU	2.3
1	A	180	ASP	2.0

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

There are no carbohydrates in this entry.

6.4 Ligands

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	CL	B	1562	1/1	0.95	0.14	-0.64	50,50,50,50	0
2	TPP	B	1557	26/26	0.99	0.10	-1.10	18,19,22,22	0
4	CL	D	1559	1/1	0.94	0.09	-1.17	32,32,32,32	0
2	TPP	A	1557	26/26	0.99	0.11	-1.17	11,20,22,24	0
2	TPP	D	1557	26/26	0.98	0.11	-1.21	9,14,17,17	0
4	CL	B	1559	1/1	0.94	0.11	-1.32	20,20,20,20	0
2	TPP	C	1557	26/26	0.99	0.10	-1.50	11,17,20,20	0
3	MN	C	1562	1/1	0.98	0.10	-1.87	22,22,22,22	0
4	CL	D	1560	1/1	0.97	0.07	-2.31	37,37,37,37	0
3	MN	B	1558	1/1	0.99	0.07	-2.36	20,20,20,20	0
3	MN	D	1558	1/1	1.00	0.07	-2.44	13,13,13,13	0
3	MN	A	1558	1/1	1.00	0.07	-3.25	19,19,19,19	0
3	MN	C	1558	1/1	1.00	0.09	-3.49	17,17,17,17	0
4	CL	A	1559	1/1	0.97	0.09	-4.20	37,37,37,37	0
4	CL	C	1561	1/1	0.98	0.06	-	23,23,23,23	0
4	CL	C	1559	1/1	0.91	0.13	-	37,37,37,37	0
4	CL	A	1561	1/1	0.98	0.19	-	13,13,13,13	0
4	CL	D	1561	1/1	0.99	0.10	-	22,22,22,22	0
4	CL	C	1560	1/1	0.99	0.07	-	31,31,31,31	0
4	CL	B	1561	1/1	0.98	0.07	-	25,25,25,25	0
4	CL	B	1560	1/1	0.99	0.10	-	25,25,25,25	0
4	CL	A	1560	1/1	0.96	0.07	-	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.