Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 10:31 AM EST

PDB ID	:	7JQ7
Title	:	The Phi-28 gp11 DNA packaging Motor
Authors	:	Morais, M.C.; White, M.A.; Dill, E.
Deposited on	:	2020-08-10
Resolution	:	2.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

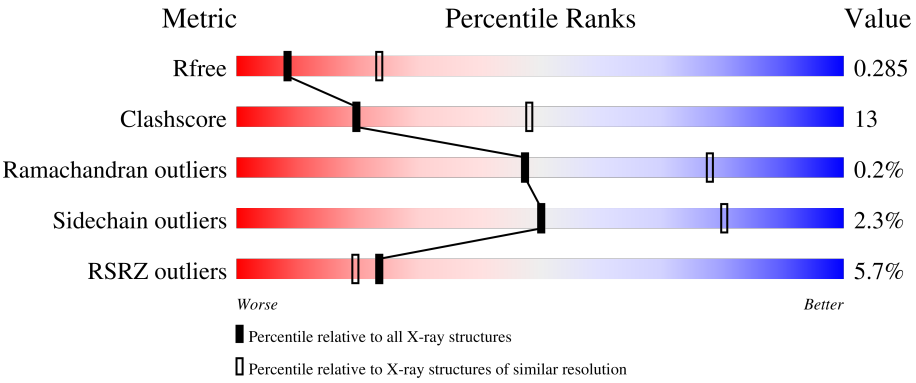
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	374	5% 71% 25%
1	B	374	4% 75% 21%
1	C	374	5% 72% 26%
1	D	374	8% 71% 26%
1	E	374	5% 70% 27%

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
2	IOD	A	405	-	-	X	-
2	IOD	A	413	-	-	X	-
2	IOD	A	429	-	-	X	-
2	IOD	B	409	-	-	X	-
2	IOD	B	413	-	-	X	-
2	IOD	B	414	-	-	X	-
2	IOD	B	428	-	-	X	-
2	IOD	C	420	-	-	X	-
2	IOD	C	434	-	-	X	-
2	IOD	D	411	-	-	X	-
2	IOD	E	412	-	-	X	-
2	IOD	E	417	-	-	X	-
2	IOD	E	419	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29824 atoms, of which 14553 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 Encapsidation protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	366	Total	C	H	N	O	S	Se	0	0	0
			5970	1967	2933	495	565	2	8			
1	B	364	Total	C	H	N	O	S	Se	0	0	0
			5957	1963	2929	493	562	2	8			
1	C	367	Total	C	H	N	O	S	Se	0	0	0
			5981	1973	2937	495	566	2	8			
1	D	364	Total	C	H	N	O	S	Se	0	0	0
			5872	1945	2869	486	562	2	8			
1	E	364	Total	C	H	N	O	S	Se	0	0	0
			5892	1949	2885	489	559	2	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	LEU	-	expression tag	UNP B1ABI1
A	368	GLU	-	expression tag	UNP B1ABI1
A	369	HIS	-	expression tag	UNP B1ABI1
A	370	HIS	-	expression tag	UNP B1ABI1
A	371	HIS	-	expression tag	UNP B1ABI1
A	372	HIS	-	expression tag	UNP B1ABI1
A	373	HIS	-	expression tag	UNP B1ABI1
A	374	HIS	-	expression tag	UNP B1ABI1
B	367	LEU	-	expression tag	UNP B1ABI1
B	368	GLU	-	expression tag	UNP B1ABI1
B	369	HIS	-	expression tag	UNP B1ABI1
B	370	HIS	-	expression tag	UNP B1ABI1
B	371	HIS	-	expression tag	UNP B1ABI1
B	372	HIS	-	expression tag	UNP B1ABI1
B	373	HIS	-	expression tag	UNP B1ABI1
B	374	HIS	-	expression tag	UNP B1ABI1
C	367	LEU	-	expression tag	UNP B1ABI1
C	368	GLU	-	expression tag	UNP B1ABI1
C	369	HIS	-	expression tag	UNP B1ABI1

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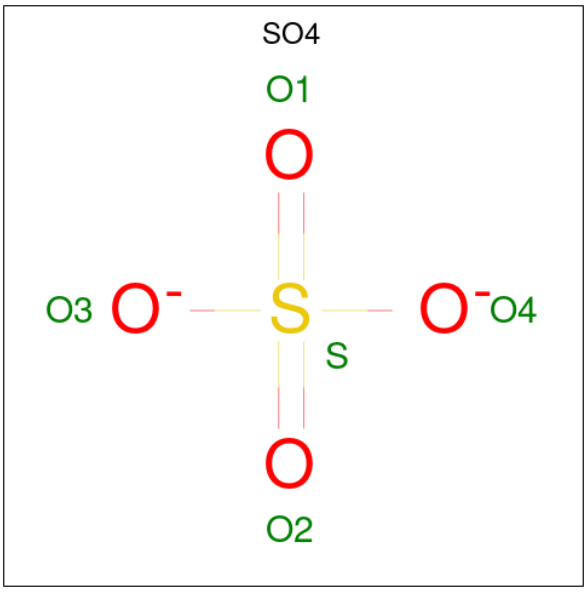
Chain	Residue	Modelled	Actual	Comment	Reference
C	370	HIS	-	expression tag	UNP B1ABI1
C	371	HIS	-	expression tag	UNP B1ABI1
C	372	HIS	-	expression tag	UNP B1ABI1
C	373	HIS	-	expression tag	UNP B1ABI1
C	374	HIS	-	expression tag	UNP B1ABI1
D	367	LEU	-	expression tag	UNP B1ABI1
D	368	GLU	-	expression tag	UNP B1ABI1
D	369	HIS	-	expression tag	UNP B1ABI1
D	370	HIS	-	expression tag	UNP B1ABI1
D	371	HIS	-	expression tag	UNP B1ABI1
D	372	HIS	-	expression tag	UNP B1ABI1
D	373	HIS	-	expression tag	UNP B1ABI1
D	374	HIS	-	expression tag	UNP B1ABI1
E	367	LEU	-	expression tag	UNP B1ABI1
E	368	GLU	-	expression tag	UNP B1ABI1
E	369	HIS	-	expression tag	UNP B1ABI1
E	370	HIS	-	expression tag	UNP B1ABI1
E	371	HIS	-	expression tag	UNP B1ABI1
E	372	HIS	-	expression tag	UNP B1ABI1
E	373	HIS	-	expression tag	UNP B1ABI1
E	374	HIS	-	expression tag	UNP B1ABI1

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total I 29 29	0	0
2	B	28	Total I 28 28	0	0
2	C	35	Total I 35 35	0	0
2	D	18	Total I 18 18	0	0
2	E	21	Total I 21 21	0	0

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



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

- Molecule 4 is water.

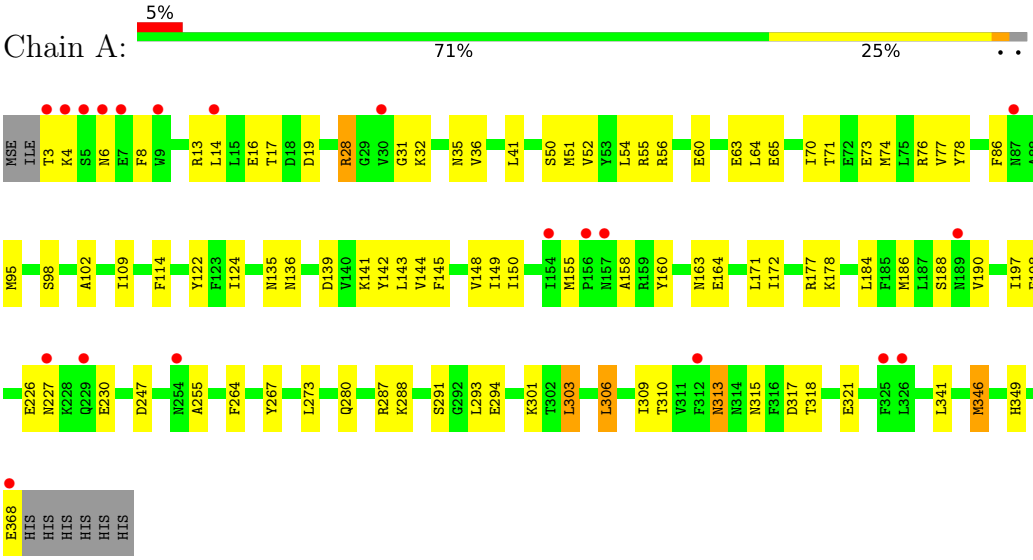
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total O 2 2	0	0
4	C	1	Total O 1 1	0	0
4	D	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

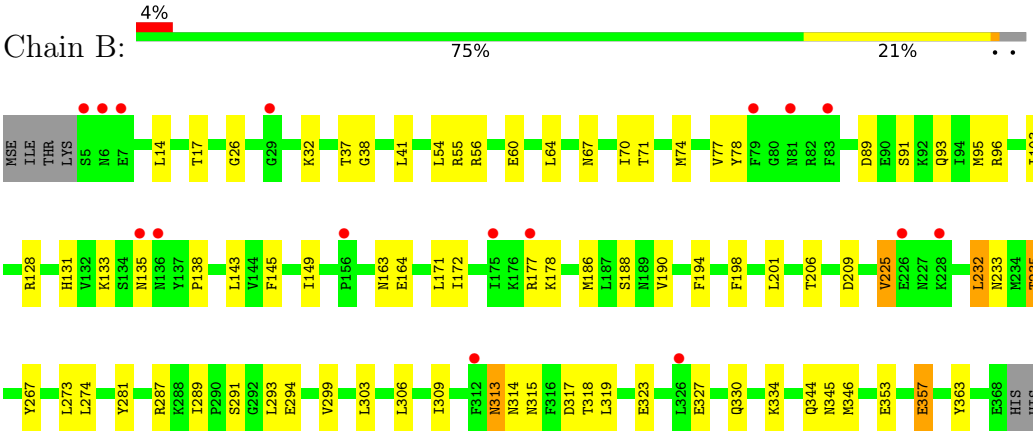
• Molecule 1: Encapsidation protein

Chain A:



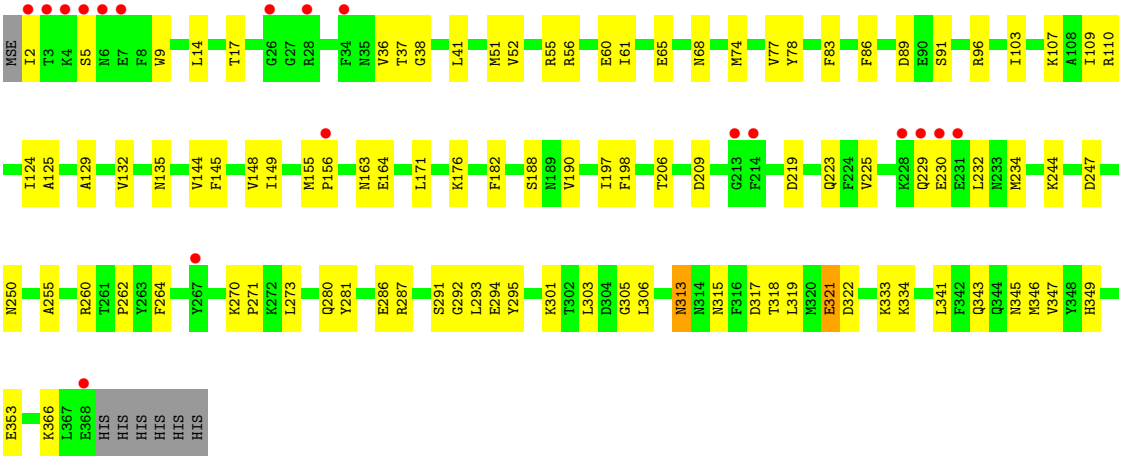
• Molecule 1: Encapsidation protein

Chain B:



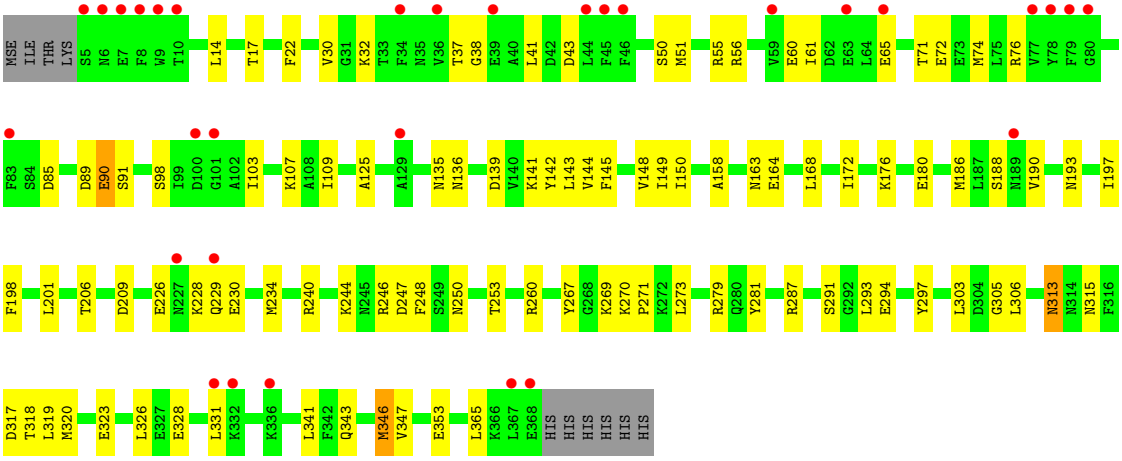
• Molecule 1: Encapsidation protein

Chain C:



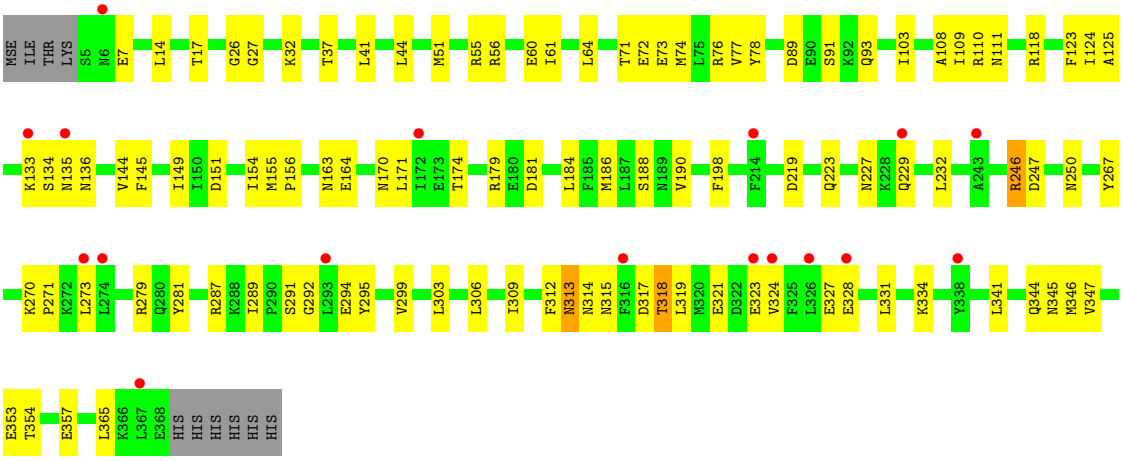
• Molecule 1: Encapsidation protein

Chain D:



• Molecule 1: Encapsidation protein

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.20Å 112.20Å 354.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.90 49.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.6 (49.69-2.90) 76.6 (49.68-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, R_{free}	0.235 , 0.284 0.237 , 0.285	Depositor DCC
R_{free} test set	2000 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	29824	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: IOD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	0/3100	0.50	0/4172
1	B	0.34	1/3091 (0.0%)	0.50	0/4158
1	C	0.32	0/3107	0.48	0/4182
1	D	0.30	0/3066	0.48	0/4132
1	E	0.30	0/3070	0.49	0/4135
All	All	0.32	1/15434 (0.0%)	0.49	0/20779

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	GLU	CG-CD	-6.55	1.42	1.51

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	3037	2933	2933	82	1
1	B	3028	2929	2930	71	1
1	C	3044	2937	2939	88	1
1	D	3003	2869	2869	82	1
1	E	3007	2885	2885	83	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	0	11	0
2	B	28	0	0	12	0
2	C	35	0	0	14	0
2	D	18	0	0	6	0
2	E	21	0	0	9	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	8	0	0	2	0
All	All	15271	14553	14556	379	3

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 13.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:OE2	1:B:178:LYS:NZ	1.86	1.08
1:C:341:LEU:HD23	1:C:346:MSE:HE3	1.35	1.04
1:A:341:LEU:HD23	1:A:346:MSE:HE3	1.41	1.03
1:D:341:LEU:HD23	1:D:346:MSE:HE3	1.41	0.98
1:A:64:LEU:HD11	2:A:413:IOD:I	2.41	0.91
1:A:287:ARG:NH1	1:A:294:GLU:OE2	2.08	0.87
1:A:70:ILE:O	1:A:95:MSE:HE1	1.75	0.86
2:A:412:IOD:I	2:A:429:IOD:I	3.33	0.85
1:D:287:ARG:NH1	1:D:294:GLU:OE2	2.11	0.84
1:E:55:ARG:NH1	1:E:60:GLU:OE1	2.11	0.83
1:B:357:GLU:OE2	2:B:409:IOD:I	2.67	0.83
1:B:37:THR:HG22	1:B:74:MSE:HE1	1.60	0.83
1:A:55:ARG:NH1	1:A:60:GLU:OE1	2.13	0.81
1:E:37:THR:HG22	1:E:74:MSE:HE1	1.63	0.80
1:C:56:ARG:NH1	1:C:164:GLU:OE2	2.14	0.80
1:A:150:ILE:HD12	1:A:160:TYR:CE1	2.17	0.80
1:E:184:LEU:HD21	1:E:186:MSE:HE3	1.64	0.80
1:C:109:ILE:HD12	1:C:110:ARG:HG2	1.61	0.80
1:E:124:ILE:HD11	1:E:171:LEU:HD21	1.65	0.79
1:B:186:MSE:HE1	1:B:201:LEU:HD21	1.63	0.78
1:D:89:ASP:OD1	1:D:91:SER:OG	2.01	0.77
1:B:287:ARG:NH1	1:B:294:GLU:OE1	2.17	0.77
1:A:219:ASP:N	1:A:219:ASP:OD2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLU:OE2	1:D:76:ARG:NH2	2.18	0.76
1:C:234:MSE:HE1	2:C:434:IOD:I	2.56	0.76
1:D:32:LYS:NZ	1:D:188:SER:O	2.18	0.76
1:D:56:ARG:NH1	1:D:164:GLU:OE2	2.21	0.74
1:E:184:LEU:HD21	1:E:186:MSE:CE	2.17	0.73
1:C:250:ASN:ND2	2:C:419:IOD:I	2.92	0.73
1:C:287:ARG:NH1	1:C:294:GLU:OE2	2.22	0.72
1:A:163:ASN:ND2	1:E:247:ASP:OD2	2.21	0.72
1:E:281:TYR:CZ	1:E:303:LEU:HD11	2.24	0.72
1:C:14:LEU:HD11	1:C:223:GLN:OE1	1.90	0.71
1:A:143:LEU:HD23	1:A:172:ILE:HD13	1.72	0.71
1:B:233:ASN:OD1	1:B:235:THR:N	2.23	0.71
1:A:51:MSE:HE3	1:A:144:VAL:HG21	1.71	0.71
1:B:55:ARG:NH1	1:B:60:GLU:OE1	2.23	0.71
1:C:51:MSE:HE3	1:C:144:VAL:HG21	1.71	0.71
1:C:41:LEU:HD11	1:C:74:MSE:HE2	1.72	0.71
1:C:225:VAL:HG23	2:C:407:IOD:I	2.61	0.71
1:D:51:MSE:HE3	1:D:144:VAL:HG21	1.71	0.71
1:E:331:LEU:HD11	1:E:365:LEU:HD23	1.73	0.71
1:A:56:ARG:NH1	1:A:164:GLU:OE2	2.23	0.70
2:D:407:IOD:I	2:D:413:IOD:I	3.50	0.70
1:B:41:LEU:HD11	1:B:74:MSE:HE2	1.74	0.70
1:B:149:ILE:HD11	1:B:198:PHE:CE1	2.27	0.69
1:A:14:LEU:O	1:A:17:THR:HG22	1.93	0.69
1:A:73:GLU:O	1:A:77:VAL:HG13	1.92	0.69
1:B:124:ILE:HD11	1:B:171:LEU:HD21	1.75	0.69
1:A:32:LYS:NZ	1:A:188:SER:O	2.26	0.68
1:D:226:GLU:HG2	2:D:411:IOD:I	2.64	0.68
1:D:247:ASP:OD2	1:E:163:ASN:ND2	2.26	0.68
1:B:225:VAL:HG23	2:B:414:IOD:I	2.64	0.68
1:A:280:GLN:OE1	1:A:301:LYS:NZ	2.24	0.67
1:C:149:ILE:HD11	1:C:198:PHE:CE1	2.29	0.67
1:D:315:ASN:OD1	1:D:317:ASP:N	2.28	0.67
1:A:357:GLU:OE2	2:A:405:IOD:I	2.83	0.67
1:D:149:ILE:HD11	1:D:198:PHE:CE1	2.30	0.66
1:A:90:GLU:O	1:B:110:ARG:NH2	2.28	0.66
1:E:357:GLU:CD	2:E:419:IOD:I	3.04	0.66
1:B:315:ASN:OD1	1:B:317:ASP:N	2.29	0.66
1:A:136:ASN:OD1	1:A:177:ARG:NH1	2.29	0.65
1:D:143:LEU:HD23	1:D:172:ILE:HD13	1.79	0.65
1:E:281:TYR:CE1	1:E:303:LEU:HD11	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:THR:CG2	1:E:74:MSE:HE1	2.26	0.65
1:E:56:ARG:NH1	1:E:164:GLU:OE2	2.30	0.65
1:C:247:ASP:OD2	1:D:163:ASN:ND2	2.29	0.64
1:C:124:ILE:HD11	1:C:171:LEU:HD21	1.79	0.64
1:D:90:GLU:OE2	1:E:110:ARG:NH2	2.30	0.64
1:C:2:ILE:HD13	1:D:176:LYS:NZ	2.12	0.64
1:E:357:GLU:OE2	2:E:419:IOD:I	2.86	0.64
1:E:26:GLY:O	1:E:32:LYS:NZ	2.25	0.63
1:B:315:ASN:HB3	1:B:318:THR:HG22	1.80	0.63
1:B:306:LEU:HB2	1:B:309:ILE:HD12	1.81	0.62
1:D:55:ARG:NH1	1:D:60:GLU:OE1	2.31	0.62
1:A:357:GLU:CD	2:A:405:IOD:I	3.08	0.62
1:E:51:MSE:HE2	1:E:144:VAL:HG21	1.81	0.62
1:D:30:VAL:HG21	1:E:133:LYS:HB2	1.82	0.62
1:A:219:ASP:OD2	2:A:418:IOD:I	2.88	0.62
1:C:190:VAL:HG12	1:C:255:ALA:HA	1.81	0.61
1:D:250:ASN:ND2	4:D:501:HOH:O	2.14	0.61
1:A:51:MSE:HE3	1:A:144:VAL:CG2	2.30	0.61
1:A:149:ILE:HD11	1:A:198:PHE:CE1	2.36	0.61
1:B:89:ASP:OD1	1:B:91:SER:OG	2.16	0.61
1:B:327:GLU:HG3	1:B:330:GLN:H	1.65	0.61
1:E:14:LEU:HD11	1:E:223:GLN:OE1	2.01	0.61
1:E:14:LEU:O	1:E:17:THR:HG22	2.00	0.61
1:B:138:PRO:HD2	2:B:413:IOD:I	2.71	0.61
1:C:96:ARG:HH12	1:C:103:ILE:HD12	1.66	0.61
1:E:149:ILE:HD11	1:E:198:PHE:CE1	2.36	0.60
1:D:180:GLU:OE1	4:D:502:HOH:O	2.16	0.60
1:B:14:LEU:O	1:B:17:THR:HG22	2.00	0.60
1:D:43:ASP:OD2	1:D:141:LYS:NZ	2.33	0.60
1:C:305:GLY:C	1:C:306:LEU:HD12	2.22	0.60
2:A:411:IOD:I	1:E:71:THR:HG21	2.72	0.60
1:C:14:LEU:O	1:C:17:THR:HG22	2.01	0.60
1:A:56:ARG:NH2	1:A:148:VAL:O	2.35	0.59
1:B:299:VAL:HG21	1:B:357:GLU:OE1	2.02	0.59
1:D:297:TYR:CE1	1:D:347:VAL:HG11	2.37	0.59
1:A:41:LEU:HD21	1:A:74:MSE:CE	2.32	0.59
1:D:313:ASN:OD1	1:D:318:THR:HG23	2.02	0.59
1:C:37:THR:HG22	1:C:74:MSE:HE1	1.85	0.59
1:A:41:LEU:HD11	1:A:74:MSE:CE	2.33	0.59
1:E:135:ASN:OD1	1:E:174:THR:HG23	2.03	0.59
1:C:38:GLY:HA2	1:C:74:MSE:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HD21	1:A:186:MSE:HE3	1.86	0.58
1:E:334:LYS:HE2	2:E:411:IOD:I	2.73	0.58
1:B:103:ILE:HD12	1:B:103:ILE:H	1.68	0.58
1:A:135:ASN:OD1	1:E:64:LEU:HD12	2.03	0.58
1:D:260:ARG:NH2	1:D:343:GLN:O	2.37	0.58
1:C:51:MSE:HE3	1:C:144:VAL:CG2	2.34	0.58
1:C:280:GLN:OE1	1:C:301:LYS:CE	2.52	0.57
1:D:14:LEU:O	1:D:17:THR:HG22	2.04	0.57
1:C:2:ILE:CG1	2:C:420:IOD:I	3.22	0.57
1:A:50:SER:N	1:A:139:ASP:O	2.36	0.57
1:D:253:THR:HA	2:D:411:IOD:I	2.74	0.57
1:C:2:ILE:HG12	2:C:420:IOD:I	2.75	0.57
1:D:61:ILE:HD12	1:D:125:ALA:HB2	1.85	0.57
1:E:331:LEU:CD1	1:E:365:LEU:HD23	2.35	0.56
1:B:225:VAL:CG2	2:B:414:IOD:I	3.23	0.56
1:D:228:LYS:O	1:D:230:GLU:N	2.38	0.56
1:A:303:LEU:HA	1:A:306:LEU:HD11	1.87	0.56
1:C:341:LEU:CD2	1:C:346:MSE:HE3	2.22	0.56
1:B:41:LEU:CD1	1:B:74:MSE:HE2	2.36	0.56
1:C:38:GLY:CA	1:C:74:MSE:HE3	2.36	0.56
1:B:128:ARG:HD2	2:B:428:IOD:I	2.77	0.55
1:B:37:THR:CG2	1:B:74:MSE:HE1	2.34	0.55
1:E:103:ILE:HD12	1:E:103:ILE:H	1.71	0.55
1:A:155:MSE:HB2	2:A:422:IOD:I	2.76	0.55
1:A:41:LEU:HD11	1:A:74:MSE:HE2	1.88	0.55
1:A:77:VAL:HG23	1:A:78:TYR:CD2	2.42	0.55
1:B:247:ASP:OD2	1:C:163:ASN:ND2	2.40	0.55
1:C:37:THR:CG2	1:C:74:MSE:HE1	2.37	0.55
1:D:51:MSE:HE3	1:D:144:VAL:CG2	2.36	0.55
1:E:344:GLN:OE1	1:E:346:MSE:HE2	2.07	0.55
1:B:38:GLY:HA2	1:B:74:MSE:HE3	1.89	0.55
1:E:188:SER:OG	1:E:190:VAL:O	2.24	0.55
1:A:90:GLU:N	1:A:90:GLU:OE1	2.41	0.54
1:D:30:VAL:HG11	1:E:134:SER:HA	1.88	0.54
1:E:341:LEU:HD23	1:E:346:MSE:HE3	1.89	0.54
1:A:124:ILE:HD11	1:A:171:LEU:HD21	1.89	0.54
1:B:206:THR:HG23	1:B:209:ASP:H	1.72	0.54
1:C:65:GLU:N	1:D:135:ASN:OD1	2.38	0.54
1:A:148:VAL:HG22	1:A:197:ILE:HG13	1.88	0.54
1:C:156:PRO:HD2	2:C:425:IOD:I	2.78	0.54
1:D:320:MSE:HB2	1:D:323:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ILE:HD12	1:E:125:ALA:HB2	1.90	0.54
1:B:70:ILE:O	1:B:95:MSE:HE1	2.08	0.54
1:C:61:ILE:HD12	1:C:125:ALA:HB2	1.89	0.54
1:E:303:LEU:HA	1:E:306:LEU:HD11	1.89	0.54
1:B:303:LEU:HA	1:B:306:LEU:HD11	1.90	0.53
1:D:148:VAL:HG22	1:D:197:ILE:HG13	1.90	0.53
1:D:71:THR:OG1	1:E:136:ASN:OD1	2.16	0.53
1:A:13:ARG:NH1	1:A:16:GLU:OE2	2.41	0.53
1:A:313:ASN:OD1	1:A:318:THR:HG23	2.09	0.53
1:C:2:ILE:HD13	1:D:176:LYS:HZ2	1.74	0.53
1:D:279:ARG:HD2	2:D:404:IOD:I	2.79	0.53
1:A:143:LEU:CD2	1:A:172:ILE:HD13	2.37	0.53
1:A:150:ILE:HD12	1:A:160:TYR:CD1	2.44	0.53
1:A:31:GLY:O	1:A:35:ASN:ND2	2.39	0.53
1:E:151:ASP:HB3	1:E:154:ILE:HD12	1.90	0.53
1:C:96:ARG:NH1	1:C:103:ILE:HD12	2.24	0.52
1:C:129:ALA:O	1:C:132:VAL:HG22	2.08	0.52
1:C:315:ASN:HB3	1:C:318:THR:HG22	1.92	0.52
1:C:280:GLN:OE1	1:C:301:LYS:HE3	2.09	0.52
1:E:315:ASN:OD1	1:E:317:ASP:N	2.40	0.52
1:B:334:LYS:NZ	2:B:418:IOD:I	3.13	0.52
1:B:38:GLY:CA	1:B:74:MSE:HE3	2.40	0.52
1:A:65:GLU:O	2:A:413:IOD:I	2.98	0.52
1:C:89:ASP:OD1	1:C:91:SER:OG	2.24	0.52
1:D:353:GLU:HB2	2:D:417:IOD:I	2.81	0.51
1:A:341:LEU:CD2	1:A:346:MSE:HE3	2.27	0.51
1:C:281:TYR:CE1	1:C:303:LEU:HD11	2.45	0.51
1:C:306:LEU:HD12	1:C:306:LEU:N	2.25	0.51
1:A:306:LEU:HB2	1:A:309:ILE:HD12	1.92	0.51
1:A:90:GLU:HB3	1:B:110:ARG:HH21	1.76	0.51
1:A:273:LEU:O	1:A:273:LEU:HD12	2.11	0.51
1:E:109:ILE:HD12	1:E:110:ARG:HB2	1.92	0.51
1:D:188:SER:OG	1:D:190:VAL:O	2.28	0.51
1:D:41:LEU:HD11	1:D:74:MSE:HE2	1.92	0.51
1:A:288:LYS:HA	1:A:293:LEU:HD23	1.94	0.51
1:B:64:LEU:HD12	1:C:135:ASN:OD1	2.11	0.51
1:C:2:ILE:HG13	2:C:420:IOD:I	2.81	0.50
1:D:244:LYS:NZ	1:E:219:ASP:OD2	2.39	0.50
1:D:141:LYS:HD3	1:D:142:TYR:CE1	2.45	0.50
1:A:89:ASP:OD1	1:A:91:SER:OG	2.22	0.50
1:B:344:GLN:CD	1:B:346:MSE:HE2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:HG23	1:B:78:TYR:CD2	2.46	0.50
1:C:5:SER:OG	1:C:230:GLU:N	2.36	0.50
1:A:63:GLU:O	1:B:131:HIS:NE2	2.45	0.50
1:B:56:ARG:NH1	1:B:164:GLU:OE2	2.44	0.50
1:D:281:TYR:CZ	1:D:303:LEU:HD11	2.46	0.49
1:C:315:ASN:OD1	1:C:317:ASP:N	2.42	0.49
1:A:267:TYR:CE1	1:A:287:ARG:HD2	2.48	0.49
1:E:327:GLU:HG2	1:E:328:GLU:N	2.28	0.49
1:A:64:LEU:CD1	2:A:413:IOD:I	3.25	0.49
1:E:7:GLU:CB	2:E:417:IOD:I	3.31	0.49
1:E:287:ARG:NH1	1:E:294:GLU:OE1	2.46	0.49
1:B:128:ARG:CD	2:B:428:IOD:I	3.30	0.49
1:E:184:LEU:CD2	1:E:186:MSE:HE3	2.39	0.49
1:B:54:LEU:HD13	1:B:124:ILE:CD1	2.42	0.49
1:C:109:ILE:HD11	1:C:110:ARG:NH1	2.27	0.49
1:A:19:ASP:OD2	1:A:221:CYS:SG	2.71	0.49
1:B:319:LEU:CD1	1:B:323:GLU:HB2	2.43	0.49
1:A:273:LEU:HD12	1:A:273:LEU:C	2.34	0.49
1:C:286:GLU:HB3	1:C:293:LEU:HD23	1.95	0.49
1:D:37:THR:HG22	1:D:74:MSE:HE1	1.95	0.49
1:E:273:LEU:C	1:E:273:LEU:HD12	2.33	0.49
1:E:327:GLU:HG2	1:E:328:GLU:H	1.78	0.49
1:C:260:ARG:NE	2:C:409:IOD:I	3.15	0.48
1:E:331:LEU:C	1:E:331:LEU:HD23	2.34	0.48
1:C:188:SER:OG	1:C:190:VAL:O	2.31	0.48
1:B:240:ARG:NH2	1:C:219:ASP:OD1	2.46	0.48
1:D:168:LEU:C	1:D:168:LEU:HD23	2.34	0.48
1:B:357:GLU:CD	2:B:409:IOD:I	3.22	0.48
1:C:9:TRP:HZ3	1:C:36:VAL:HG23	1.79	0.48
1:E:77:VAL:HG23	1:E:78:TYR:CD2	2.48	0.48
1:E:299:VAL:CG2	1:E:354:THR:HG22	2.44	0.48
1:D:267:TYR:CE1	1:D:287:ARG:HD2	2.48	0.48
1:E:41:LEU:HD21	1:E:74:MSE:HE2	1.96	0.48
1:E:306:LEU:HD12	1:E:306:LEU:O	2.14	0.48
1:A:98:SER:HA	1:A:102:ALA:O	2.14	0.47
1:C:366:LYS:NZ	2:C:431:IOD:I	3.16	0.47
1:A:54:LEU:HD13	1:A:124:ILE:CD1	2.44	0.47
1:D:315:ASN:HB3	1:D:318:THR:HG22	1.97	0.47
1:B:306:LEU:O	1:B:306:LEU:HD12	2.15	0.47
1:C:41:LEU:CD1	1:C:74:MSE:HE2	2.44	0.47
1:C:273:LEU:C	1:C:273:LEU:HD12	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:HB3	1:C:319:LEU:HD13	1.97	0.47
1:A:184:LEU:HD21	1:A:186:MSE:CE	2.45	0.47
1:C:321:GLU:HG3	1:C:322:ASP:H	1.79	0.47
1:B:41:LEU:CG	1:B:74:MSE:HE2	2.45	0.47
1:E:124:ILE:CD1	1:E:171:LEU:HD21	2.42	0.47
1:E:93:GLN:NE2	1:E:108:ALA:O	2.42	0.47
1:A:188:SER:OG	1:A:190:VAL:O	2.31	0.46
1:D:326:LEU:HD11	1:D:331:LEU:HB3	1.96	0.46
1:D:281:TYR:CZ	1:D:303:LEU:CD1	2.98	0.46
1:E:273:LEU:HD12	1:E:273:LEU:O	2.15	0.46
1:A:86:PHE:CD1	1:A:86:PHE:C	2.89	0.46
1:B:299:VAL:HG11	1:B:357:GLU:OE1	2.14	0.46
1:C:2:ILE:HD13	1:D:176:LYS:HZ1	1.80	0.46
1:B:38:GLY:N	1:B:74:MSE:HE3	2.31	0.46
1:B:267:TYR:CE1	1:B:287:ARG:HD2	2.51	0.46
1:E:32:LYS:NZ	1:E:188:SER:O	2.48	0.46
1:A:306:LEU:CB	1:A:309:ILE:HD12	2.46	0.46
1:C:234:MSE:CE	2:C:434:IOD:I	3.33	0.46
1:B:124:ILE:HA	2:B:428:IOD:I	2.85	0.46
1:C:295:TYR:HB2	1:C:347:VAL:HG12	1.98	0.46
1:E:27:GLY:CA	1:E:227:ASN:HD21	2.28	0.46
1:D:85:ASP:HB3	1:D:98:SER:HB3	1.98	0.46
1:A:178:LYS:O	1:A:178:LYS:HG3	2.16	0.45
1:B:313:ASN:OD1	1:B:318:THR:HG23	2.16	0.45
1:B:344:GLN:OE1	1:B:346:MSE:HE2	2.16	0.45
1:C:55:ARG:NH1	1:C:60:GLU:OE1	2.47	0.45
1:D:90:GLU:HB3	1:E:109:ILE:CD1	2.47	0.45
1:D:107:LYS:HE2	1:D:109:ILE:HG21	1.97	0.45
1:E:179:ARG:NH2	1:E:181:ASP:O	2.42	0.45
1:E:306:LEU:HB2	1:E:309:ILE:HD12	1.98	0.45
1:C:56:ARG:NH2	1:C:148:VAL:O	2.49	0.45
1:C:264:PHE:HA	1:C:349:HIS:O	2.16	0.45
1:A:3:THR:HG22	1:A:4:LYS:N	2.32	0.45
1:B:133:LYS:HA	2:B:419:IOD:I	2.87	0.45
1:C:280:GLN:HG2	1:C:301:LYS:HD3	1.98	0.45
1:D:103:ILE:N	1:D:103:ILE:HD12	2.32	0.45
1:A:54:LEU:HD13	1:A:124:ILE:HD11	1.99	0.45
1:C:262:PRO:HG2	1:C:264:PHE:CZ	2.52	0.45
1:D:37:THR:CG2	1:D:74:MSE:HE1	2.46	0.45
1:A:3:THR:HG22	1:A:4:LYS:H	1.82	0.44
1:A:226:GLU:OE2	2:A:415:IOD:I	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:OD1	1:C:318:THR:HG23	2.16	0.44
1:B:143:LEU:HD23	1:B:172:ILE:HD13	1.99	0.44
1:B:274:LEU:HD11	1:B:306:LEU:HD13	1.99	0.44
1:C:110:ARG:O	1:C:110:ARG:HG3	2.17	0.44
1:C:281:TYR:CZ	1:C:303:LEU:CD1	3.01	0.44
1:D:341:LEU:HD23	1:D:346:MSE:CE	2.29	0.44
1:E:313:ASN:OD1	1:E:318:THR:HG23	2.17	0.44
1:B:289:ILE:HD13	1:B:294:GLU:HG3	1.99	0.44
1:D:90:GLU:HB3	1:E:109:ILE:HD11	1.99	0.44
1:D:150:ILE:HG21	1:D:158:ALA:HB3	2.00	0.44
1:D:193:ASN:HB2	1:D:260:ARG:O	2.18	0.44
1:A:109:ILE:HG13	1:A:114:PHE:HE1	1.82	0.44
1:A:150:ILE:HD12	1:A:160:TYR:CZ	2.53	0.44
1:C:232:LEU:HD12	1:C:232:LEU:N	2.32	0.44
1:C:77:VAL:HG23	1:C:78:TYR:CD2	2.53	0.44
1:A:124:ILE:CD1	1:A:171:LEU:HD21	2.48	0.43
1:D:273:LEU:HD12	1:D:273:LEU:C	2.39	0.43
1:C:206:THR:HG23	1:C:209:ASP:H	1.83	0.43
1:D:281:TYR:CE1	1:D:303:LEU:HD11	2.53	0.43
1:D:306:LEU:N	1:D:306:LEU:HD12	2.33	0.43
1:D:353:GLU:HG2	2:D:405:IOD:I	2.88	0.43
1:E:72:GLU:OE2	1:E:76:ARG:NH2	2.48	0.43
1:D:305:GLY:C	1:D:306:LEU:HD12	2.39	0.43
1:D:143:LEU:CD2	1:D:172:ILE:HD13	2.47	0.43
1:C:280:GLN:OE1	1:C:301:LYS:NZ	2.52	0.43
1:D:246:ARG:CZ	1:D:250:ASN:HD21	2.32	0.43
1:D:273:LEU:HD12	1:D:273:LEU:O	2.18	0.43
1:E:295:TYR:HB2	1:E:347:VAL:HG12	1.99	0.43
1:A:247:ASP:OD2	1:B:163:ASN:ND2	2.51	0.43
1:A:264:PHE:HA	1:A:349:HIS:O	2.18	0.43
1:B:353:GLU:HB2	2:B:426:IOD:I	2.89	0.43
1:E:44:LEU:O	1:E:118:ARG:NH2	2.42	0.43
1:E:312:PHE:CD1	1:E:324:VAL:CG2	3.02	0.43
1:B:274:LEU:CD1	1:B:306:LEU:HD13	2.49	0.43
1:D:14:LEU:HD23	1:D:22:PHE:CD1	2.54	0.43
1:D:143:LEU:HD23	1:D:172:ILE:CD1	2.47	0.43
1:E:51:MSE:HE2	1:E:144:VAL:CG2	2.48	0.43
1:E:89:ASP:OD1	1:E:91:SER:OG	2.27	0.43
1:E:229:GLN:CB	1:E:232:LEU:HD11	2.48	0.43
1:A:3:THR:HG23	1:B:178:LYS:HE3	2.01	0.42
1:A:190:VAL:HG23	1:A:255:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:HA	1:B:363:TYR:OH	2.20	0.42
1:E:279:ARG:CZ	2:E:416:IOD:I	3.38	0.42
1:E:111:ASN:HB3	1:E:123:PHE:O	2.20	0.42
1:C:333:LYS:HD3	1:C:334:LYS:HZ2	1.84	0.42
1:B:67:ASN:HB2	1:B:93:GLN:HG2	2.02	0.42
1:B:273:LEU:HD12	1:B:273:LEU:C	2.39	0.42
1:C:353:GLU:HG2	2:C:401:IOD:I	2.89	0.42
1:D:38:GLY:N	1:D:74:MSE:HE3	2.35	0.42
1:B:281:TYR:CZ	1:B:303:LEU:CD1	3.03	0.42
1:C:51:MSE:HG2	1:C:52:VAL:N	2.35	0.42
1:C:148:VAL:O	1:C:148:VAL:HG22	2.19	0.42
1:E:73:GLU:O	1:E:77:VAL:HG13	2.19	0.42
1:E:313:ASN:HD22	1:E:314:ASN:N	2.18	0.42
1:A:184:LEU:CD2	1:A:186:MSE:HE3	2.49	0.42
1:B:26:GLY:O	1:B:32:LYS:NZ	2.39	0.42
1:D:313:ASN:HB3	1:D:319:LEU:HD13	2.02	0.42
1:C:148:VAL:HG22	1:C:197:ILE:HG13	2.01	0.42
1:D:206:THR:HG23	1:D:209:ASP:H	1.84	0.42
1:A:141:LYS:HD3	1:A:142:TYR:CE1	2.55	0.41
1:A:310:THR:OG1	2:A:429:IOD:I	2.98	0.41
1:A:315:ASN:OD1	1:A:317:ASP:N	2.50	0.41
1:C:38:GLY:N	1:C:74:MSE:HE3	2.35	0.41
1:A:32:LYS:O	1:A:36:VAL:HG23	2.20	0.41
1:A:52:VAL:HG22	1:A:122:TYR:HB2	2.02	0.41
1:D:267:TYR:OH	1:D:269:LYS:HG3	2.19	0.41
1:D:365:LEU:HD12	1:D:365:LEU:N	2.34	0.41
1:D:141:LYS:HD3	1:D:142:TYR:CZ	2.55	0.41
1:E:267:TYR:CE1	1:E:287:ARG:HD2	2.55	0.41
1:B:54:LEU:HD13	1:B:124:ILE:HD11	2.01	0.41
1:C:155:MSE:SE	2:C:422:IOD:I	3.58	0.41
1:D:90:GLU:OE1	1:E:109:ILE:HD11	2.20	0.41
1:E:7:GLU:HG3	2:E:417:IOD:I	2.90	0.41
1:A:28:ARG:HE	1:A:227:ASN:ND2	2.18	0.41
1:A:155:MSE:HG3	1:A:158:ALA:HB2	2.02	0.41
1:B:71:THR:HA	1:B:95:MSE:HE1	2.03	0.41
1:B:138:PRO:CD	2:B:413:IOD:I	3.39	0.41
1:D:328:GLU:OE1	1:D:331:LEU:HD21	2.20	0.41
1:E:155:MSE:HB3	2:E:412:IOD:I	2.90	0.41
1:D:270:LYS:HB3	1:D:271:PRO:HD2	2.03	0.41
1:C:260:ARG:NH2	1:C:343:GLN:O	2.43	0.41
1:E:111:ASN:HB3	1:E:123:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:SER:O	2:C:424:IOD:I	3.09	0.41
1:C:281:TYR:CE2	1:C:303:LEU:CD1	3.04	0.41
1:D:234:MSE:O	1:D:240:ARG:HD3	2.21	0.41
1:E:156:PRO:HD2	2:E:412:IOD:I	2.90	0.41
1:E:289:ILE:HG13	1:E:292:GLY:H	1.85	0.41
1:E:353:GLU:HG2	2:E:419:IOD:I	2.91	0.41
1:D:50:SER:N	1:D:139:ASP:O	2.54	0.41
1:E:246:ARG:CZ	1:E:250:ASN:HD22	2.34	0.41
1:B:188:SER:OG	1:B:190:VAL:O	2.33	0.40
1:B:240:ARG:NE	1:C:219:ASP:OD1	2.54	0.40
1:C:83:PHE:CZ	1:C:86:PHE:HB2	2.56	0.40
1:A:178:LYS:O	1:A:178:LYS:CG	2.69	0.40
1:A:365:LEU:N	1:A:365:LEU:HD12	2.36	0.40
1:C:176:LYS:HB2	1:C:182:PHE:CE1	2.56	0.40
1:C:292:GLY:C	1:C:293:LEU:HD12	2.41	0.40
1:C:321:GLU:CG	1:C:322:ASP:H	2.33	0.40
1:D:65:GLU:OE1	1:E:110:ARG:NH1	2.55	0.40
1:D:248:PHE:CE1	1:E:170:ASN:OD1	2.74	0.40
1:E:319:LEU:HD12	1:E:323:GLU:HB2	2.03	0.40
1:A:148:VAL:O	1:A:148:VAL:HG22	2.20	0.40
1:B:232:LEU:N	1:B:232:LEU:CD1	2.85	0.40
1:C:107:LYS:HE2	1:C:109:ILE:HG21	2.03	0.40
1:C:244:LYS:NZ	2:C:414:IOD:I	3.24	0.40
1:C:270:LYS:HB3	1:C:271:PRO:HD2	2.04	0.40
1:B:313:ASN:HD22	1:B:314:ASN:N	2.19	0.40
1:C:68:ASN:ND2	1:D:136:ASN:O	2.50	0.40
1:D:186:MSE:HE1	1:D:201:LEU:HD21	2.02	0.40
1:E:270:LYS:HB3	1:E:271:PRO:HD2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LEU:O	1:E:291:SER:OG[7_555]	1.99	0.21
1:A:291:SER:OG	1:C:293:LEU:O[7_555]	2.02	0.18
1:B:291:SER:OG	1:B:293:LEU:O[7_555]	2.12	0.08

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	364/374 (97%)	353 (97%)	10 (3%)	1 (0%)	41 71
1	B	362/374 (97%)	351 (97%)	11 (3%)	0	100 100
1	C	365/374 (98%)	356 (98%)	8 (2%)	1 (0%)	41 71
1	D	362/374 (97%)	354 (98%)	7 (2%)	1 (0%)	41 71
1	E	362/374 (97%)	352 (97%)	10 (3%)	0	100 100
All	All	1815/1870 (97%)	1766 (97%)	46 (2%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	GLU
1	A	321	GLU
1	D	229	GLN

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	327/335 (98%)	315 (96%)	12 (4%)	34 68
1	B	326/335 (97%)	317 (97%)	9 (3%)	43 76
1	C	327/335 (98%)	322 (98%)	5 (2%)	65 87
1	D	321/335 (96%)	316 (98%)	5 (2%)	62 86
1	E	321/335 (96%)	315 (98%)	6 (2%)	57 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1622/1675 (97%)	1585 (98%)	37 (2%)	50 80

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	8	PHE
1	A	28	ARG
1	A	71	THR
1	A	76	ARG
1	A	145	PHE
1	A	219	ASP
1	A	303	LEU
1	A	306	LEU
1	A	313	ASN
1	A	346	MSE
1	A	368	GLU
1	B	96	ARG
1	B	135	ASN
1	B	145	PHE
1	B	177	ARG
1	B	225	VAL
1	B	232	LEU
1	B	235	THR
1	B	313	ASN
1	B	345	ASN
1	C	145	PHE
1	C	229	GLN
1	C	291	SER
1	C	313	ASN
1	C	345	ASN
1	D	90	GLU
1	D	145	PHE
1	D	291	SER
1	D	313	ASN
1	D	346	MSE
1	E	145	PHE
1	E	246	ARG
1	E	313	ASN
1	E	318	THR
1	E	321	GLU
1	E	345	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	344	GLN
1	E	227	ASN
1	E	280	GLN
1	E	313	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 133 ligands modelled in this entry, 131 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	436	-	4,4,4	0.16	0	6,6,6	0.24	0
3	SO4	E	422	-	4,4,4	0.15	0	6,6,6	0.06	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.

No monomer is involved in short contacts.

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	358/374 (95%)	0.41	20 (5%)	24	20	22, 51, 94, 125	0
1	B	356/374 (95%)	0.40	16 (4%)	33	29	18, 51, 90, 133	0
1	C	359/374 (95%)	0.33	18 (5%)	28	25	24, 50, 84, 119	0
1	D	356/374 (95%)	0.65	31 (8%)	10	7	31, 67, 111, 165	0
1	E	356/374 (95%)	0.35	17 (4%)	30	27	26, 55, 94, 133	0
All	All	1785/1870 (95%)	0.43	102 (5%)	23	19	18, 54, 101, 165	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	ASN	17.5
1	B	6	ASN	12.1
1	B	5	SER	10.9
1	C	229	GLN	9.5
1	D	5	SER	9.4
1	A	156	PRO	8.4
1	A	3	THR	8.1
1	B	7	GLU	7.3
1	C	3	THR	6.6
1	A	5	SER	6.6
1	A	6	ASN	5.8
1	D	7	GLU	5.7
1	A	7	GLU	5.3
1	B	29	GLY	5.2
1	D	9	TRP	5.2
1	C	230	GLU	4.8
1	C	7	GLU	4.8
1	C	5	SER	4.8
1	B	326	LEU	4.7
1	D	36	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	331	LEU	4.2
1	B	135	ASN	4.1
1	A	154	ILE	4.0
1	E	229	GLN	4.0
1	D	8	PHE	3.9
1	C	214	PHE	3.8
1	D	367	LEU	3.8
1	D	79	PHE	3.8
1	E	274	LEU	3.6
1	D	78	TYR	3.5
1	C	368	GLU	3.5
1	E	324	VAL	3.5
1	D	45	PHE	3.5
1	D	332	LYS	3.4
1	E	214	PHE	3.1
1	C	6	ASN	3.0
1	D	34	PHE	3.0
1	D	77	VAL	2.9
1	D	368	GLU	2.9
1	D	227	ASN	2.9
1	E	316	PHE	2.8
1	E	367	LEU	2.8
1	C	4	LYS	2.8
1	D	10	THR	2.8
1	D	46	PHE	2.8
1	A	229	GLN	2.7
1	C	2	ILE	2.7
1	E	326	LEU	2.6
1	A	157	ASN	2.6
1	A	9	TRP	2.6
1	D	39	GLU	2.6
1	C	231	GLU	2.5
1	D	83	PHE	2.5
1	E	323	GLU	2.5
1	D	80	GLY	2.5
1	A	4	LYS	2.5
1	B	83	PHE	2.5
1	D	44	LEU	2.5
1	A	30	VAL	2.5
1	A	14	LEU	2.5
1	D	229	GLN	2.4
1	A	312	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	81	ASN	2.4
1	B	79	PHE	2.3
1	B	228	LYS	2.3
1	B	136	ASN	2.3
1	C	156	PRO	2.3
1	B	312	PHE	2.3
1	E	133	LYS	2.3
1	E	293	LEU	2.3
1	B	177	ARG	2.3
1	D	336	LYS	2.3
1	E	135	ASN	2.3
1	B	175	ILE	2.3
1	E	172	ILE	2.3
1	A	254	ASN	2.2
1	A	368	GLU	2.2
1	D	63	GLU	2.2
1	A	326	LEU	2.2
1	B	156	PRO	2.2
1	C	228	LYS	2.2
1	D	189	ASN	2.2
1	D	65	GLU	2.2
1	E	328	GLU	2.2
1	B	226	GLU	2.2
1	A	227	ASN	2.2
1	D	129	ALA	2.2
1	A	87	ASN	2.1
1	E	6	ASN	2.1
1	C	28	ARG	2.1
1	D	101	GLY	2.1
1	E	338	TYR	2.1
1	E	273	LEU	2.1
1	C	267	TYR	2.1
1	C	213	GLY	2.1
1	A	189	ASN	2.1
1	D	100	ASP	2.0
1	E	243	ALA	2.0
1	A	325	PHE	2.0
1	D	59	VAL	2.0
1	C	34	PHE	2.0
1	C	26	GLY	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
2	IOD	B	414	1/1	0.22	0.19	127,127,127,127	1
2	IOD	B	424	1/1	0.47	0.25	187,187,187,187	0
2	IOD	C	425	1/1	0.48	0.14	145,145,145,145	1
2	IOD	A	422	1/1	0.56	0.11	147,147,147,147	1
2	IOD	C	433	1/1	0.67	0.12	127,127,127,127	1
2	IOD	E	420	1/1	0.67	0.10	124,124,124,124	0
2	IOD	B	428	1/1	0.79	0.16	139,139,139,139	1
2	IOD	A	429	1/1	0.80	0.19	113,113,113,113	1
2	IOD	C	432	1/1	0.80	0.13	130,130,130,130	1
2	IOD	C	429	1/1	0.81	0.11	132,132,132,132	0
2	IOD	D	413	1/1	0.82	0.10	146,146,146,146	1
2	IOD	D	414	1/1	0.82	0.10	127,127,127,127	1
2	IOD	B	422	1/1	0.82	0.12	124,124,124,124	1
2	IOD	C	434	1/1	0.83	0.12	138,138,138,138	1
2	IOD	A	426	1/1	0.83	0.12	80,80,80,80	1
2	IOD	D	418	1/1	0.84	0.13	118,118,118,118	1
2	IOD	B	409	1/1	0.86	0.11	57,57,57,57	1
2	IOD	C	428	1/1	0.86	0.14	101,101,101,101	1
2	IOD	E	418	1/1	0.87	0.07	150,150,150,150	1
2	IOD	E	416	1/1	0.87	0.22	133,133,133,133	1
2	IOD	B	418	1/1	0.88	0.06	102,102,102,102	1
2	IOD	A	413	1/1	0.88	0.12	116,116,116,116	1
2	IOD	B	419	1/1	0.89	0.07	126,126,126,126	1
2	IOD	C	419	1/1	0.89	0.14	107,107,107,107	0
2	IOD	C	431	1/1	0.89	0.15	136,136,136,136	1
2	IOD	B	427	1/1	0.89	0.13	149,149,149,149	1
2	IOD	E	421	1/1	0.89	0.07	101,101,101,101	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	C	420	1/1	0.90	0.11	104,104,104,104	1
2	IOD	B	423	1/1	0.90	0.21	124,124,124,124	1
2	IOD	D	409	1/1	0.90	0.13	128,128,128,128	0
2	IOD	E	415	1/1	0.90	0.08	122,122,122,122	1
2	IOD	A	428	1/1	0.91	0.15	170,170,170,170	0
2	IOD	A	423	1/1	0.91	0.07	78,78,78,78	1
2	IOD	B	420	1/1	0.91	0.06	88,88,88,88	1
2	IOD	D	411	1/1	0.91	0.09	114,114,114,114	1
2	IOD	C	424	1/1	0.92	0.11	110,110,110,110	1
2	IOD	E	411	1/1	0.92	0.08	81,81,81,81	1
2	IOD	E	417	1/1	0.92	0.10	96,96,96,96	1
2	IOD	E	414	1/1	0.93	0.05	87,87,87,87	1
2	IOD	B	426	1/1	0.93	0.09	123,123,123,123	1
2	IOD	C	435	1/1	0.93	0.08	100,100,100,100	1
2	IOD	D	406	1/1	0.93	0.06	100,100,100,100	1
2	IOD	D	408	1/1	0.93	0.17	58,58,58,58	1
2	IOD	B	417	1/1	0.93	0.15	88,88,88,88	1
2	IOD	E	412	1/1	0.93	0.08	63,63,63,63	1
2	IOD	C	426	1/1	0.94	0.08	84,84,84,84	1
2	IOD	D	410	1/1	0.94	0.07	116,116,116,116	1
2	IOD	A	419	1/1	0.94	0.08	101,101,101,101	1
2	IOD	D	412	1/1	0.94	0.08	99,99,99,99	1
2	IOD	D	405	1/1	0.95	0.09	74,74,74,74	1
2	IOD	B	407	1/1	0.95	0.06	68,68,68,68	1
2	IOD	B	416	1/1	0.95	0.09	131,131,131,131	0
2	IOD	C	418	1/1	0.95	0.05	93,93,93,93	1
2	IOD	E	401	1/1	0.95	0.06	56,56,56,56	1
2	IOD	A	421	1/1	0.95	0.07	100,100,100,100	1
2	IOD	B	421	1/1	0.95	0.09	85,85,85,85	1
2	IOD	A	420	1/1	0.96	0.07	80,80,80,80	1
2	IOD	A	418	1/1	0.96	0.10	94,94,94,94	1
2	IOD	D	417	1/1	0.96	0.09	107,107,107,107	1
2	IOD	A	427	1/1	0.96	0.04	114,114,114,114	1
2	IOD	B	410	1/1	0.96	0.06	84,84,84,84	1
2	IOD	A	409	1/1	0.96	0.12	70,70,70,70	1
2	IOD	C	430	1/1	0.96	0.04	119,119,119,119	0
3	SO4	C	436	5/5	0.96	0.18	29,31,33,37	5
3	SO4	E	422	5/5	0.96	0.11	59,60,61,62	0
2	IOD	A	406	1/1	0.97	0.05	52,52,52,52	1
2	IOD	B	425	1/1	0.97	0.05	82,82,82,82	1
2	IOD	D	404	1/1	0.97	0.15	58,58,58,58	1
2	IOD	E	405	1/1	0.97	0.08	70,70,70,70	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	E	410	1/1	0.97	0.05	72,72,72,72	1
2	IOD	B	411	1/1	0.97	0.10	87,87,87,87	1
2	IOD	A	416	1/1	0.97	0.07	88,88,88,88	1
2	IOD	E	413	1/1	0.97	0.07	94,94,94,94	1
2	IOD	D	407	1/1	0.97	0.07	80,80,80,80	1
2	IOD	C	427	1/1	0.97	0.05	110,110,110,110	0
2	IOD	B	415	1/1	0.97	0.09	83,83,83,83	0
2	IOD	C	411	1/1	0.97	0.12	78,78,78,78	0
2	IOD	C	415	1/1	0.97	0.08	56,56,56,56	1
2	IOD	E	419	1/1	0.97	0.06	64,64,64,64	1
2	IOD	C	417	1/1	0.97	0.04	101,101,101,101	0
2	IOD	B	408	1/1	0.97	0.15	65,65,65,65	1
2	IOD	A	417	1/1	0.97	0.05	87,87,87,87	0
2	IOD	D	416	1/1	0.97	0.07	100,100,100,100	1
2	IOD	C	407	1/1	0.98	0.07	64,64,64,64	1
2	IOD	C	409	1/1	0.98	0.13	46,46,46,46	1
2	IOD	B	401	1/1	0.98	0.07	63,63,63,63	1
2	IOD	C	413	1/1	0.98	0.12	57,57,57,57	1
2	IOD	B	402	1/1	0.98	0.09	59,59,59,59	1
2	IOD	E	406	1/1	0.98	0.06	81,81,81,81	1
2	IOD	E	407	1/1	0.98	0.06	80,80,80,80	1
2	IOD	E	408	1/1	0.98	0.07	73,73,73,73	1
2	IOD	E	409	1/1	0.98	0.08	75,75,75,75	1
2	IOD	C	416	1/1	0.98	0.07	80,80,80,80	1
2	IOD	D	401	1/1	0.98	0.16	34,34,34,34	1
2	IOD	B	403	1/1	0.98	0.07	54,54,54,54	1
2	IOD	B	404	1/1	0.98	0.09	49,49,49,49	1
2	IOD	A	405	1/1	0.98	0.10	51,51,51,51	1
2	IOD	A	415	1/1	0.98	0.10	62,62,62,62	1
2	IOD	C	423	1/1	0.98	0.12	67,67,67,67	1
2	IOD	A	403	1/1	0.98	0.04	75,75,75,75	1
2	IOD	A	425	1/1	0.98	0.07	67,67,67,67	1
2	IOD	A	407	1/1	0.98	0.11	68,68,68,68	1
2	IOD	A	408	1/1	0.98	0.06	76,76,76,76	1
2	IOD	A	404	1/1	0.98	0.07	53,53,53,53	1
2	IOD	A	412	1/1	0.98	0.08	58,58,58,58	1
2	IOD	D	415	1/1	0.98	0.11	61,61,61,61	1
2	IOD	C	410	1/1	0.99	0.05	68,68,68,68	1
2	IOD	A	410	1/1	0.99	0.10	70,70,70,70	1
2	IOD	C	412	1/1	0.99	0.16	62,62,62,62	0
2	IOD	E	402	1/1	0.99	0.04	63,63,63,63	1
2	IOD	E	403	1/1	0.99	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	E	404	1/1	0.99	0.13	49,49,49,49	1
2	IOD	B	412	1/1	0.99	0.15	61,61,61,61	1
2	IOD	C	414	1/1	0.99	0.12	95,95,95,95	0
2	IOD	B	413	1/1	0.99	0.09	40,40,40,40	1
2	IOD	A	411	1/1	0.99	0.10	62,62,62,62	1
2	IOD	D	402	1/1	0.99	0.08	67,67,67,67	1
2	IOD	D	403	1/1	0.99	0.09	65,65,65,65	1
2	IOD	B	405	1/1	0.99	0.07	54,54,54,54	1
2	IOD	B	406	1/1	0.99	0.10	64,64,64,64	1
2	IOD	A	402	1/1	0.99	0.13	52,52,52,52	1
2	IOD	A	401	1/1	0.99	0.08	35,35,35,35	1
2	IOD	C	421	1/1	0.99	0.06	63,63,63,63	1
2	IOD	C	422	1/1	0.99	0.05	97,97,97,97	1
2	IOD	C	401	1/1	0.99	0.09	59,59,59,59	1
2	IOD	C	403	1/1	0.99	0.10	57,57,57,57	1
2	IOD	C	404	1/1	0.99	0.10	53,53,53,53	1
2	IOD	C	405	1/1	0.99	0.09	52,52,52,52	1
2	IOD	C	406	1/1	0.99	0.04	49,49,49,49	1
2	IOD	A	424	1/1	0.99	0.10	59,59,59,59	0
2	IOD	A	414	1/1	0.99	0.05	68,68,68,68	1
2	IOD	C	402	1/1	1.00	0.12	32,32,32,32	1
2	IOD	C	408	1/1	1.00	0.10	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.