Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:25 AM GMT

PDB ID	:	3OXN
Title	:	The crystal structure of a putative transcriptional regulator from Vibrio parahaemolyticus
Authors	:	Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-09-21
Resolution	:	2.70 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:

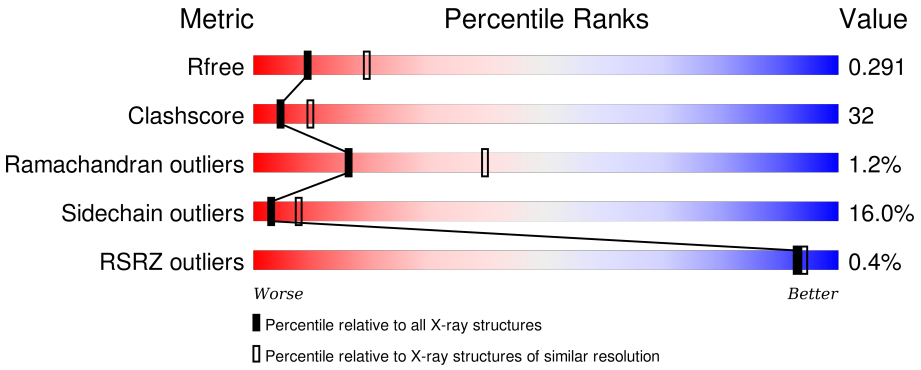
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	241	37% 41% 9% • 12%
1	B	241	37% 41% 10% • 11%
1	C	241	40% 40% 8% 12%
1	D	241	44% 37% 8% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6886 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 Putative transcriptional regulator, LysR family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	Se	0	0	0
			1697	1092	288	307	5	5			
1	B	215	Total	C	N	O	S	Se	0	1	0
			1719	1107	289	313	5	5			
1	C	213	Total	C	N	O	S	Se	0	0	0
			1702	1095	287	310	5	5			
1	D	212	Total	C	N	O	S	Se	0	0	0
			1681	1080	286	305	5	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	MSE	-	INITIATING METHIONINE	UNP Q87TP2
A	331	GLU	-	EXPRESSION TAG	UNP Q87TP2
A	332	GLY	-	EXPRESSION TAG	UNP Q87TP2
A	333	HIS	-	EXPRESSION TAG	UNP Q87TP2
A	334	HIS	-	EXPRESSION TAG	UNP Q87TP2
A	335	HIS	-	EXPRESSION TAG	UNP Q87TP2
A	336	HIS	-	EXPRESSION TAG	UNP Q87TP2
A	337	HIS	-	EXPRESSION TAG	UNP Q87TP2
A	338	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	98	MSE	-	INITIATING METHIONINE	UNP Q87TP2
B	331	GLU	-	EXPRESSION TAG	UNP Q87TP2
B	332	GLY	-	EXPRESSION TAG	UNP Q87TP2
B	333	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	334	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	335	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	336	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	337	HIS	-	EXPRESSION TAG	UNP Q87TP2
B	338	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	98	MSE	-	INITIATING METHIONINE	UNP Q87TP2
C	331	GLU	-	EXPRESSION TAG	UNP Q87TP2
C	332	GLY	-	EXPRESSION TAG	UNP Q87TP2

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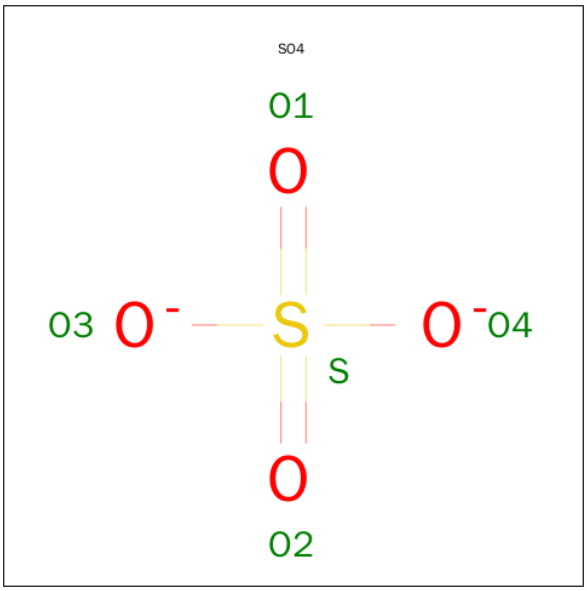
Chain	Residue	Modelled	Actual	Comment	Reference
C	333	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	334	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	335	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	336	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	337	HIS	-	EXPRESSION TAG	UNP Q87TP2
C	338	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	98	MSE	-	INITIATING METHIONINE	UNP Q87TP2
D	331	GLU	-	EXPRESSION TAG	UNP Q87TP2
D	332	GLY	-	EXPRESSION TAG	UNP Q87TP2
D	333	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	334	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	335	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	336	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	337	HIS	-	EXPRESSION TAG	UNP Q87TP2
D	338	HIS	-	EXPRESSION TAG	UNP Q87TP2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0

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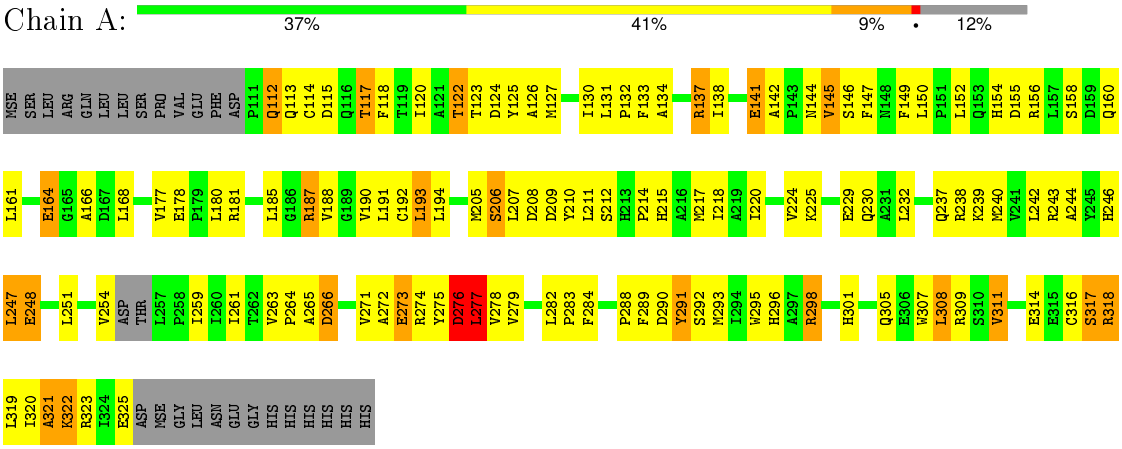
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	25	Total O 25 25	0	0
3	C	15	Total O 15 15	0	0
3	D	15	Total O 15 15	0	0

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.

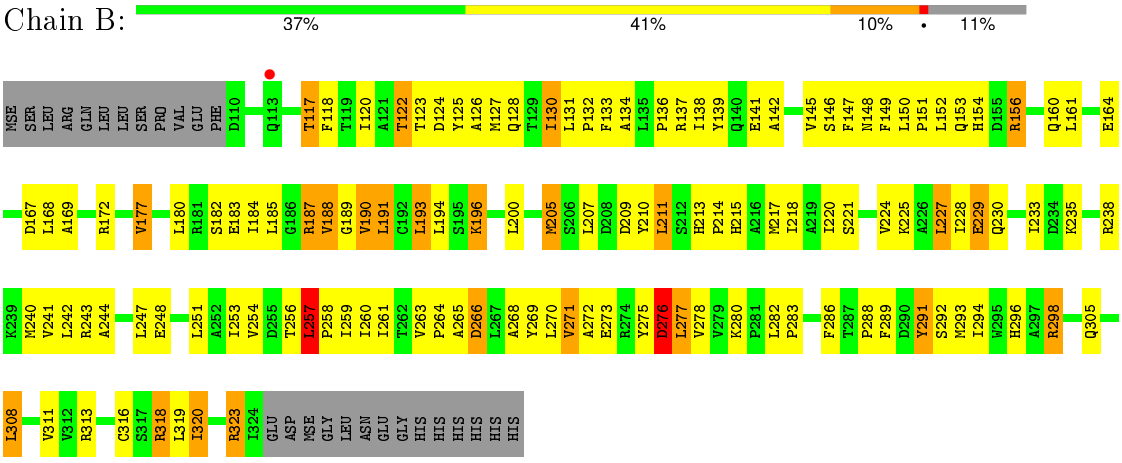
- Molecule 1: Putative transcriptional regulator, LysR family

Chain A:



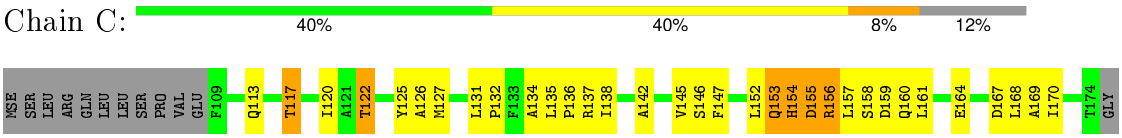
- Molecule 1: Putative transcriptional regulator, LysR family

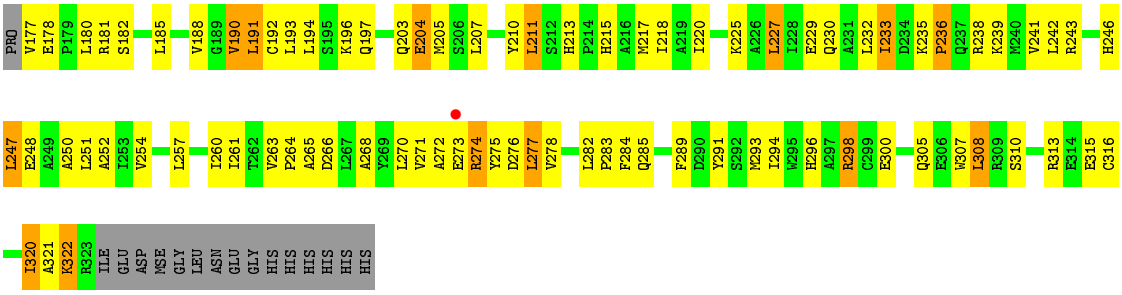
Chain B:



- Molecule 1: Putative transcriptional regulator, LysR family

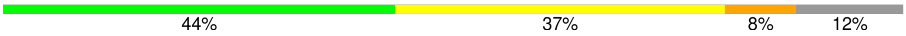
Chain C:

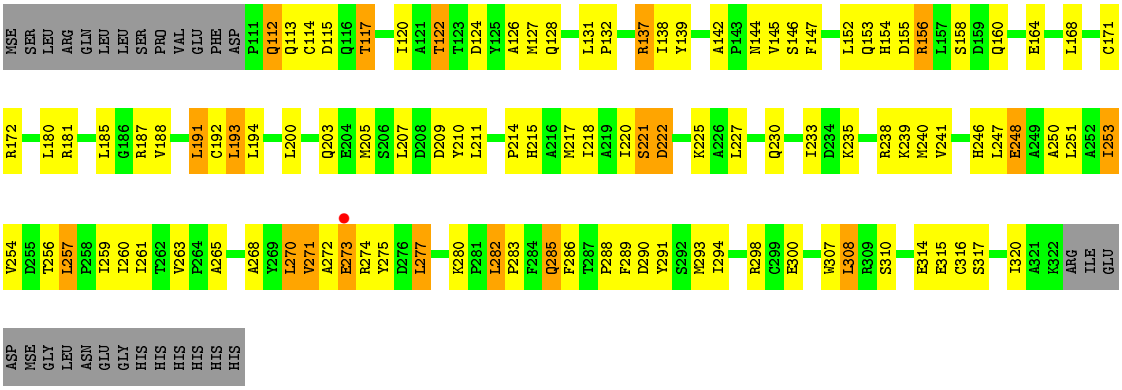




- Molecule 1: Putative transcriptional regulator, LysR family

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.32Å 50.49Å 108.12Å 86.19° 82.89° 86.74°	Depositor
Resolution (Å)	38.91 – 2.70 47.45 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.5 (38.91-2.70) 89.8 (47.45-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.245 , 0.290 0.246 , 0.291	Depositor DCC
R_{free} test set	1431 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.0	EDS
Estimated twinning fraction	0.065 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 38221 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6886	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 6.62% 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: 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	0.44	0/1733	0.65	1/2353 (0.0%)
1	B	0.51	0/1760	0.67	0/2394
1	C	0.46	1/1738 (0.1%)	0.60	0/2361
1	D	0.45	0/1718	0.62	0/2336
All	All	0.46	1/6949 (0.0%)	0.64	1/9444 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	CYS	CB-SG	-5.47	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	LEU	CA-CB-CG	5.09	127.01	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	1697	0	1710	111	0
1	B	1719	0	1726	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1702	0	1704	107	0
1	D	1681	0	1686	100	0
2	D	5	0	0	1	0
3	A	27	0	0	3	0
3	B	25	0	0	4	0
3	C	15	0	0	1	0
3	D	15	0	0	0	0
All	All	6886	0	6826	438	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 32.

All (438) 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:318:ARG:HG2	1:A:318:ARG:HH21	1.09	1.13
1:B:318:ARG:HH11	1:B:318:ARG:HG2	1.13	1.12
1:B:177:VAL:HG23	1:B:180:LEU:HB2	1.28	1.07
1:B:217:MSE:HE1	1:B:225:LYS:HG2	1.13	1.07
1:D:247:LEU:HD11	1:D:271:VAL:HG11	1.41	1.03
1:B:117:THR:HB	1:B:146:SER:HB3	1.46	0.97
1:C:247:LEU:HD11	1:C:271:VAL:HG11	1.50	0.94
1:A:160:GLN:HA	1:A:164:GLU:HG3	1.49	0.93
1:A:137:ARG:HH21	1:A:318:ARG:HD2	1.34	0.93
1:A:124:ASP:OD2	1:D:246:HIS:HE1	1.51	0.92
1:B:190:VAL:HG12	1:B:282:LEU:HD11	1.54	0.89
1:B:272:ALA:HA	1:B:277:LEU:HD22	1.55	0.87
1:A:218:ILE:HG21	1:A:247:LEU:HB3	1.57	0.87
1:A:272:ALA:HA	1:A:277:LEU:HD22	1.56	0.87
1:B:272:ALA:HA	1:B:277:LEU:CD2	2.05	0.86
1:B:133:PHE:CD1	1:B:319:LEU:HD13	2.11	0.86
1:B:256:THR:O	1:B:257:LEU:HB2	1.73	0.86
1:A:318:ARG:NH2	1:A:318:ARG:HG2	1.89	0.86
1:B:217:MSE:HE1	1:B:225:LYS:CG	2.04	0.85
1:C:271:VAL:HG13	1:C:275:TYR:HD2	1.41	0.85
1:D:253:ILE:HD12	1:D:259:ILE:HD13	1.59	0.84
1:B:217:MSE:CE	1:B:225:LYS:HG2	2.05	0.84
1:C:271:VAL:HG13	1:C:275:TYR:CD2	2.14	0.83
1:A:194:LEU:O	1:A:277:LEU:HB2	1.79	0.83
1:A:272:ALA:HA	1:A:277:LEU:CD2	2.09	0.82
1:D:271:VAL:HG13	1:D:275:TYR:HD2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:THR:HG22	1:D:126:ALA:HB3	1.63	0.80
1:B:218:ILE:HG21	1:B:247:LEU:HB3	1.63	0.80
1:A:137:ARG:HH21	1:A:318:ARG:CD	1.95	0.79
1:C:271:VAL:O	1:C:274:ARG:HG3	1.83	0.78
1:C:122:THR:HG22	1:C:126:ALA:HB3	1.63	0.77
1:D:256:THR:HG22	1:D:257:LEU:HD23	1.66	0.77
1:B:207:LEU:HD21	1:B:235:LYS:HD2	1.66	0.77
1:B:122:THR:HG22	1:B:126:ALA:HB3	1.67	0.77
1:A:168:LEU:HD11	1:A:293:MSE:HB3	1.68	0.76
1:B:318:ARG:HG2	1:B:318:ARG:NH1	1.92	0.75
1:B:194:LEU:O	1:B:277:LEU:HB2	1.86	0.75
1:B:205:MSE:HE2	1:B:280:LYS:HB2	1.67	0.74
1:A:240:MSE:HE1	1:A:243:ARG:HB2	1.70	0.73
1:A:134:ALA:O	1:A:138:ILE:HG12	1.88	0.72
1:B:210:TYR:HB2	1:B:283:PRO:HG3	1.71	0.72
1:B:133:PHE:CD1	1:B:319:LEU:CD1	2.72	0.72
1:A:210:TYR:HB2	1:A:283:PRO:HG2	1.72	0.72
1:D:271:VAL:HG13	1:D:275:TYR:CD2	2.25	0.71
1:D:194:LEU:O	1:D:277:LEU:HB2	1.90	0.71
1:D:251:LEU:O	1:D:254:VAL:HG22	1.91	0.71
1:A:124:ASP:OD2	1:D:246:HIS:CE1	2.42	0.71
1:C:194:LEU:O	1:C:277:LEU:HB2	1.90	0.70
1:A:246:HIS:HD2	1:D:127:MSE:HB3	1.56	0.70
1:C:113:GLN:NE2	1:D:113:GLN:HG2	2.07	0.70
1:A:137:ARG:NH2	1:A:318:ARG:HD2	2.07	0.70
1:B:185:LEU:HD21	1:B:293:MSE:HG3	1.73	0.69
1:D:285:GLN:CD	1:D:285:GLN:H	1.93	0.69
1:B:127:MSE:HG2	1:C:246:HIS:CD2	2.28	0.69
1:A:318:ARG:CG	1:A:318:ARG:HH21	1.97	0.69
1:D:218:ILE:HG21	1:D:247:LEU:HB3	1.73	0.69
1:B:187:ARG:HG2	1:B:288:PRO:HB2	1.75	0.68
1:A:190:VAL:HG12	1:A:282:LEU:HD11	1.73	0.68
1:B:318:ARG:HH11	1:B:318:ARG:CG	1.97	0.68
1:A:271:VAL:HB	1:A:275:TYR:CD2	2.29	0.68
1:B:193:LEU:HA	1:B:278:VAL:O	1.95	0.67
1:A:188:VAL:HB	1:A:289:PHE:CE1	2.28	0.67
1:B:138:ILE:HG21	1:B:147:PHE:CE2	2.29	0.67
1:D:181:ARG:HD3	1:D:300:GLU:OE1	1.96	0.66
1:B:130:ILE:O	1:B:133:PHE:HB3	1.94	0.66
1:C:248:GLU:HA	1:C:251:LEU:HD12	1.78	0.66
1:A:215:HIS:CD2	1:A:238:ARG:HD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ALA:HA	1:C:277:LEU:CD2	2.25	0.65
1:A:320:ILE:HG23	1:A:323:ARG:NH2	2.11	0.65
1:C:181:ARG:HD3	1:C:300:GLU:OE1	1.97	0.65
1:C:207:LEU:HD21	1:C:235:LYS:HG3	1.77	0.65
1:C:185:LEU:HD21	1:C:293:MSE:HG3	1.78	0.64
1:B:214:PRO:HB2	1:B:259:ILE:HG22	1.79	0.64
1:C:296:HIS:ND1	1:C:298:ARG:HB3	2.12	0.64
1:C:272:ALA:HA	1:C:277:LEU:HD21	1.79	0.64
1:A:296:HIS:ND1	1:A:298:ARG:HB3	2.12	0.64
1:B:137:ARG:NH2	1:B:311:VAL:HG12	2.13	0.64
1:B:211:LEU:HD23	1:B:211:LEU:C	2.19	0.63
1:A:214:PRO:HA	1:A:239:LYS:HG3	1.81	0.62
1:D:142:ALA:HB1	1:D:145:VAL:HG13	1.81	0.62
1:D:138:ILE:HG21	1:D:147:PHE:CZ	2.34	0.62
1:D:230:GLN:HA	1:D:230:GLN:NE2	2.15	0.62
1:D:122:THR:HB	1:D:127:MSE:HG2	1.82	0.62
1:A:271:VAL:HB	1:A:275:TYR:HD2	1.62	0.62
1:B:124:ASP:OD2	1:C:246:HIS:CE1	2.53	0.61
1:B:125:TYR:CD1	1:B:264:PRO:HB2	2.35	0.61
1:B:160:GLN:HA	1:B:164:GLU:HG3	1.81	0.61
1:C:125:TYR:CE1	1:C:264:PRO:HB2	2.34	0.61
1:A:217:MSE:SE	1:A:225:LYS:HG2	2.50	0.61
1:B:188:VAL:HB	1:B:289:PHE:CE1	2.35	0.61
1:D:271:VAL:O	1:D:274:ARG:HG2	2.00	0.61
1:B:247:LEU:HD11	1:B:271:VAL:HG21	1.83	0.60
1:A:193:LEU:HG	1:A:277:LEU:HD21	1.84	0.60
1:B:133:PHE:CE1	1:B:319:LEU:CD1	2.83	0.60
1:A:246:HIS:HD2	1:D:127:MSE:CB	2.13	0.60
1:D:248:GLU:HA	1:D:251:LEU:HD12	1.83	0.60
1:C:251:LEU:O	1:C:254:VAL:HG22	2.01	0.60
1:C:117:THR:HB	1:C:146:SER:HB3	1.82	0.60
1:B:254:VAL:HG23	1:B:261:ILE:HD11	1.84	0.60
1:A:308:LEU:O	1:A:311:VAL:HG23	2.02	0.60
1:D:314:GLU:O	1:D:317:SER:HB2	2.02	0.60
1:B:217:MSE:HE3	1:B:220:ILE:HB	1.82	0.60
1:C:131:LEU:HD21	1:C:170:ILE:HD12	1.84	0.60
1:C:158:SER:HA	1:C:180:LEU:HD11	1.84	0.60
1:D:154:HIS:NE2	2:D:1:SO4:O4	2.35	0.59
1:B:224:VAL:HA	1:B:227:LEU:HD22	1.83	0.59
1:B:194:LEU:HD21	1:B:260:ILE:HG23	1.84	0.59
1:B:133:PHE:CG	1:B:319:LEU:HD13	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CD1	1:A:319:LEU:HD13	2.38	0.59
1:C:125:TYR:CE1	1:C:264:PRO:CB	2.86	0.59
1:B:318:ARG:NH1	1:B:318:ARG:CG	2.61	0.59
1:A:138:ILE:HG21	1:A:147:PHE:CE2	2.37	0.59
1:B:269:TYR:O	1:B:273:GLU:HB2	2.01	0.59
1:B:133:PHE:O	1:B:136:PRO:HD2	2.02	0.59
1:A:214:PRO:HB2	1:A:259:ILE:HG22	1.84	0.59
1:A:321:ALA:O	1:A:325:GLU:HG2	2.03	0.59
1:D:152:LEU:HD13	1:D:171:CYS:HB3	1.84	0.59
1:A:118:PHE:HE1	1:A:145:VAL:CG2	2.16	0.59
1:B:225:LYS:NZ	1:B:229:GLU:OE1	2.35	0.58
1:B:200:LEU:HD13	1:B:205:MSE:HG2	1.86	0.58
1:C:125:TYR:HE1	1:C:264:PRO:HB2	1.69	0.57
1:D:239:LYS:HG2	1:D:241:VAL:HG23	1.86	0.57
1:A:137:ARG:O	1:A:141:GLU:HB2	2.04	0.57
1:B:215:HIS:CE1	1:B:238:ARG:HD2	2.39	0.57
1:C:217:MSE:CE	1:C:220:ILE:HG21	2.35	0.57
1:C:142:ALA:HB1	1:C:145:VAL:HG13	1.87	0.57
1:A:130:ILE:O	1:A:133:PHE:HB3	2.04	0.57
1:A:307:TRP:O	1:A:311:VAL:HG22	2.05	0.56
1:B:142:ALA:HB1	1:B:145:VAL:HG13	1.85	0.56
1:D:122:THR:CG2	1:D:126:ALA:HB3	2.35	0.56
1:B:147:PHE:HB2	1:C:242:LEU:HD12	1.87	0.56
1:D:168:LEU:HD11	1:D:293:MSE:HB3	1.87	0.56
1:C:230:GLN:HA	1:C:230:GLN:NE2	2.20	0.56
1:B:133:PHE:CE1	1:B:319:LEU:HD12	2.40	0.56
1:D:187:ARG:HG2	1:D:290:ASP:OD1	2.05	0.56
1:B:323:ARG:HH11	1:B:323:ARG:HG2	1.71	0.56
1:C:239:LYS:HG3	1:C:241:VAL:HG23	1.88	0.56
1:B:266:ASP:HB3	1:B:323:ARG:HH12	1.69	0.56
1:C:142:ALA:O	1:C:145:VAL:HG22	2.06	0.56
1:C:134:ALA:O	1:C:138:ILE:HG12	2.06	0.56
1:C:218:ILE:HG21	1:C:247:LEU:HB3	1.88	0.55
1:B:184:ILE:HA	1:B:292:SER:HB3	1.87	0.55
1:C:167:ASP:HB3	1:C:305:GLN:OE1	2.05	0.55
1:A:187:ARG:HG2	1:A:288:PRO:HB2	1.87	0.55
1:B:190:VAL:CG1	1:B:282:LEU:HD11	2.33	0.55
1:A:191:LEU:HB2	1:A:265:ALA:HA	1.87	0.55
1:B:190:VAL:HG12	1:B:282:LEU:CD1	2.33	0.55
1:D:207:LEU:HD21	1:D:235:LYS:HG3	1.88	0.55
1:A:138:ILE:HG21	1:A:147:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:HG3	1:A:274:ARG:N	2.20	0.55
1:C:196:LYS:HD2	1:C:276:ASP:HB3	1.88	0.55
1:D:138:ILE:HG21	1:D:147:PHE:CE2	2.41	0.55
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.72	0.55
1:A:190:VAL:CG1	1:A:282:LEU:HD11	2.36	0.54
1:D:246:HIS:HB3	1:D:248:GLU:HG2	1.89	0.54
1:A:206:SER:HB3	1:A:209:ASP:OD1	2.07	0.54
1:C:218:ILE:HB	1:C:263:VAL:HG12	1.89	0.54
1:D:272:ALA:HA	1:D:277:LEU:HD22	1.90	0.54
1:A:120:ILE:HD11	1:A:308:LEU:HD11	1.89	0.54
1:D:217:MSE:HE3	1:D:240:MSE:HE1	1.90	0.54
1:A:314:GLU:O	1:A:318:ARG:HB2	2.08	0.53
1:B:193:LEU:HD22	1:B:263:VAL:HG21	1.89	0.53
1:C:117:THR:CB	1:C:146:SER:HB3	2.39	0.53
1:B:293:MSE:O	1:B:294:ILE:HD13	2.08	0.53
1:C:213:HIS:HB2	1:C:260:ILE:CD1	2.39	0.53
1:B:134:ALA:O	1:B:138:ILE:HG12	2.07	0.53
1:B:296:HIS:ND1	1:B:298:ARG:HB3	2.23	0.53
1:C:194:LEU:HB2	1:C:278:VAL:HG22	1.91	0.53
1:B:120:ILE:HD11	1:B:308:LEU:HD11	1.91	0.53
1:C:320:ILE:HG22	1:C:321:ALA:N	2.23	0.53
1:C:113:GLN:HE22	1:D:113:GLN:HG2	1.74	0.52
1:D:215:HIS:CE1	1:D:238:ARG:HD2	2.44	0.52
1:B:254:VAL:HG23	1:B:261:ILE:CD1	2.40	0.52
1:A:161:LEU:HA	1:A:166:ALA:HB3	1.92	0.52
1:A:194:LEU:HD11	1:A:205:MSE:CE	2.38	0.52
1:B:217:MSE:HE3	1:B:220:ILE:CG2	2.40	0.52
1:C:247:LEU:CD1	1:C:271:VAL:HG11	2.32	0.52
1:A:320:ILE:HG23	1:A:323:ARG:HH22	1.75	0.52
1:A:181:ARG:HD3	3:A:73:HOH:O	2.09	0.52
1:D:117:THR:HA	1:D:146:SER:O	2.10	0.52
1:B:185:LEU:HD13	1:B:316:CYS:SG	2.50	0.51
1:B:177:VAL:HG13	3:B:37:HOH:O	2.10	0.51
1:B:217:MSE:HE3	1:B:220:ILE:CB	2.40	0.51
1:B:221:SER:OG	1:B:224:VAL:HG23	2.10	0.51
1:A:217:MSE:HE3	1:A:240:MSE:SE	2.61	0.51
1:B:137:ARG:HH21	1:B:311:VAL:HG12	1.73	0.51
1:C:177:VAL:O	1:C:180:LEU:HB2	2.10	0.51
1:B:183:GLU:OE1	1:B:313:ARG:NH1	2.42	0.51
1:C:125:TYR:CD1	1:C:264:PRO:HG2	2.46	0.51
1:A:158:SER:HA	1:A:180:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ILE:O	1:D:221:SER:CB	2.59	0.51
1:B:220:ILE:HG22	1:B:221:SER:O	2.10	0.51
1:C:188:VAL:HB	1:C:289:PHE:CE1	2.45	0.51
1:D:247:LEU:CD1	1:D:271:VAL:HG11	2.28	0.51
1:D:230:GLN:O	1:D:233:ILE:HB	2.10	0.51
1:B:218:ILE:HG21	1:B:247:LEU:CB	2.38	0.51
1:B:123:THR:O	1:B:127:MSE:HB2	2.10	0.51
1:B:142:ALA:O	1:B:145:VAL:HG22	2.11	0.51
1:D:158:SER:HA	1:D:180:LEU:HD21	1.93	0.51
1:D:160:GLN:HA	1:D:164:GLU:HB2	1.92	0.50
1:B:168:LEU:HD11	1:B:293:MSE:HB3	1.94	0.50
1:C:211:LEU:HD21	1:C:235:LYS:HB3	1.92	0.50
1:C:191:LEU:HB2	1:C:265:ALA:HA	1.93	0.50
1:A:120:ILE:HB	1:A:149:PHE:CD1	2.46	0.50
1:C:182:SER:HB2	1:C:294:ILE:HD13	1.92	0.50
1:D:307:TRP:O	1:D:310:SER:OG	2.27	0.50
1:D:193:LEU:HG	1:D:277:LEU:HD21	1.92	0.50
1:C:235:LYS:O	1:C:236:PRO:O	2.29	0.50
1:C:207:LEU:HD13	1:C:284:PHE:HB3	1.93	0.50
1:C:138:ILE:HG21	1:C:147:PHE:CE2	2.46	0.50
1:C:125:TYR:HD1	1:C:264:PRO:HG2	1.76	0.50
1:B:126:ALA:HB2	1:B:291:TYR:HE2	1.77	0.50
1:A:133:PHE:CG	1:A:319:LEU:HD13	2.47	0.50
1:C:313:ARG:NH2	3:C:49:HOH:O	2.41	0.50
1:B:257:LEU:O	1:B:259:ILE:N	2.43	0.49
1:C:211:LEU:HD23	1:C:236:PRO:HD2	1.94	0.49
1:C:215:HIS:CE1	1:C:238:ARG:HD2	2.47	0.49
1:B:126:ALA:HA	1:B:130:ILE:HG13	1.94	0.49
1:A:271:VAL:O	1:A:272:ALA:C	2.51	0.49
1:D:257:LEU:N	1:D:257:LEU:HD23	2.27	0.49
1:B:196:LYS:HG3	1:B:276:ASP:OD1	2.12	0.49
1:C:263:VAL:CG2	1:C:268:ALA:HB2	2.43	0.49
1:D:205:MSE:HE3	1:D:283:PRO:HG3	1.94	0.49
1:C:307:TRP:O	1:C:310:SER:OG	2.26	0.48
1:B:177:VAL:HG21	1:B:182:SER:HB3	1.96	0.48
1:B:254:VAL:HA	1:B:259:ILE:HD11	1.94	0.48
1:D:168:LEU:HD12	1:D:294:ILE:O	2.13	0.48
1:B:225:LYS:HG3	1:B:243:ARG:NH1	2.28	0.48
1:A:156:ARG:NH1	1:A:164:GLU:OE2	2.45	0.48
1:A:248:GLU:HA	1:A:251:LEU:HD12	1.96	0.48
1:A:193:LEU:HD22	1:A:263:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:O	1:A:215:HIS:HE1	1.97	0.48
1:B:193:LEU:C	1:B:194:LEU:HD23	2.34	0.48
1:B:244:ALA:HB1	1:C:127:MSE:CE	2.43	0.48
1:D:217:MSE:HE1	1:D:238:ARG:HH21	1.78	0.48
1:D:193:LEU:HG	1:D:277:LEU:CD2	2.43	0.48
1:D:271:VAL:HG12	1:D:272:ALA:N	2.29	0.48
1:D:117:THR:CG2	1:D:146:SER:HB2	2.43	0.48
1:B:123:THR:HG1	1:B:291:TYR:HH	1.60	0.48
1:D:158:SER:OG	1:D:180:LEU:HD11	2.14	0.48
1:B:149:PHE:HE2	1:C:242:LEU:HD11	1.78	0.48
1:D:217:MSE:SE	1:D:225:LYS:HG2	2.64	0.48
1:C:120:ILE:HD11	1:C:308:LEU:HD11	1.94	0.47
1:B:138:ILE:HG21	1:B:147:PHE:CZ	2.49	0.47
1:C:117:THR:CG2	1:C:146:SER:HB3	2.45	0.47
1:A:254:VAL:HG23	1:A:261:ILE:HD11	1.95	0.47
1:B:153:GLN:HG2	1:C:153:GLN:HE21	1.79	0.47
1:A:193:LEU:HD11	1:A:272:ALA:HB2	1.97	0.47
1:B:266:ASP:N	1:B:266:ASP:OD2	2.47	0.47
1:A:273:GLU:CG	1:A:274:ARG:N	2.78	0.47
1:B:218:ILE:CD1	1:B:244:ALA:HB3	2.43	0.47
1:B:177:VAL:HG23	1:B:180:LEU:CB	2.20	0.47
1:C:227:LEU:O	1:C:230:GLN:HB3	2.14	0.47
1:C:155:ASP:N	1:C:155:ASP:OD2	2.48	0.47
1:D:137:ARG:HG3	1:D:315:GLU:OE2	2.15	0.47
1:D:194:LEU:HD21	1:D:260:ILE:HG12	1.95	0.47
1:D:272:ALA:HA	1:D:277:LEU:CD2	2.45	0.47
1:B:205:MSE:HE2	1:B:280:LYS:CB	2.40	0.47
1:B:139:TYR:CE1	1:C:241:VAL:HG13	2.49	0.47
1:C:204:GLU:OE2	1:C:204:GLU:HA	2.14	0.47
1:D:193:LEU:HD22	1:D:263:VAL:HG21	1.97	0.47
1:C:160:GLN:HA	1:C:164:GLU:HB2	1.96	0.47
1:D:153:GLN:CB	1:D:156:ARG:HG3	2.45	0.47
1:A:301:HIS:CD2	3:A:77:HOH:O	2.66	0.47
1:A:210:TYR:CB	1:A:283:PRO:HG2	2.42	0.47
1:B:125:TYR:CD1	1:B:264:PRO:CB	2.98	0.47
1:D:275:TYR:HB2	1:D:277:LEU:HD13	1.95	0.47
1:A:156:ARG:NH2	1:A:164:GLU:OE2	2.45	0.47
1:A:194:LEU:HD11	1:A:205:MSE:HE3	1.97	0.46
1:C:235:LYS:HE3	1:C:236:PRO:CD	2.45	0.46
1:A:244:ALA:HB1	1:D:127:MSE:HE1	1.97	0.46
1:B:253:ILE:HG13	1:B:259:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LEU:HD12	1:C:157:LEU:O	2.16	0.46
1:B:191:LEU:HB2	1:B:265:ALA:HA	1.97	0.46
1:D:117:THR:HB	1:D:146:SER:HB2	1.97	0.46
1:A:261:ILE:HD12	1:A:261:ILE:N	2.31	0.46
1:A:230:GLN:HA	1:A:230:GLN:NE2	2.30	0.46
1:D:139:TYR:HE1	1:D:145:VAL:O	1.97	0.46
1:C:117:THR:HA	1:C:146:SER:O	2.15	0.46
1:B:200:LEU:CD1	1:B:209:ASP:HB3	2.46	0.46
1:A:181:ARG:HB2	1:A:295:TRP:CE2	2.51	0.46
1:D:171:CYS:SG	1:D:172:ARG:N	2.88	0.46
1:A:207:LEU:HA	1:A:283:PRO:HB2	1.98	0.46
1:A:117:THR:HB	1:A:146:SER:HB3	1.98	0.46
1:A:318:ARG:NH2	1:A:318:ARG:CG	2.64	0.46
1:A:115:ASP:C	1:A:115:ASP:OD1	2.54	0.46
1:D:200:LEU:HD11	1:D:209:ASP:HB3	1.97	0.46
1:B:319:LEU:O	1:B:323:ARG:HB2	2.16	0.45
1:C:117:THR:HG22	1:C:146:SER:HB3	1.97	0.45
1:A:185:LEU:HD13	1:A:316:CYS:SG	2.57	0.45
1:B:230:GLN:NE2	1:B:233:ILE:HD13	2.31	0.45
1:D:142:ALA:HB1	1:D:145:VAL:CG1	2.46	0.45
1:B:189:GLY:O	1:B:265:ALA:N	2.30	0.45
1:A:161:LEU:HD12	1:A:180:LEU:HD13	1.98	0.45
1:D:112:GLN:HG2	1:D:112:GLN:H	1.42	0.45
1:B:138:ILE:HG21	1:B:147:PHE:HE2	1.79	0.45
1:B:217:MSE:HG2	1:B:220:ILE:HG13	1.98	0.45
1:C:241:VAL:HG21	1:C:257:LEU:HD23	1.99	0.45
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.82	0.45
1:B:131:LEU:O	1:B:132:PRO:C	2.53	0.45
1:A:218:ILE:O	1:A:220:ILE:HG12	2.16	0.45
1:B:210:TYR:CB	1:B:283:PRO:HG3	2.43	0.45
1:A:177:VAL:O	1:A:180:LEU:HB2	2.16	0.45
1:D:270:LEU:HD22	1:D:270:LEU:O	2.17	0.45
1:B:182:SER:HB2	1:B:294:ILE:HD13	1.99	0.45
1:A:248:GLU:H	1:A:248:GLU:HG2	1.54	0.45
1:A:122:THR:OG1	1:A:126:ALA:HB3	2.17	0.45
1:B:122:THR:CG2	1:B:126:ALA:HB3	2.41	0.45
1:B:200:LEU:HD11	1:B:209:ASP:HB3	1.99	0.45
1:C:217:MSE:HE2	1:C:220:ILE:HG21	1.98	0.45
1:A:207:LEU:O	1:A:208:ASP:C	2.54	0.44
1:D:273:GLU:HG2	1:D:273:GLU:H	1.59	0.44
1:A:125:TYR:CD1	1:A:264:PRO:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:NE2	1:A:238:ARG:HD2	2.32	0.44
1:D:139:TYR:CE1	1:D:145:VAL:O	2.70	0.44
1:B:248:GLU:HA	1:B:251:LEU:HD12	1.99	0.44
1:B:272:ALA:HA	1:B:277:LEU:HD21	1.97	0.44
1:A:210:TYR:O	1:A:215:HIS:CE1	2.70	0.44
1:C:217:MSE:HE1	1:C:225:LYS:HA	1.99	0.44
1:D:188:VAL:HB	1:D:289:PHE:CE1	2.53	0.44
1:C:152:LEU:HD23	1:C:154:HIS:HA	1.99	0.44
1:A:240:MSE:HB3	1:A:240:MSE:HE3	1.78	0.44
1:A:224:VAL:HG11	1:A:289:PHE:CE2	2.52	0.44
1:D:239:LYS:HE2	1:D:241:VAL:CG2	2.47	0.44
1:D:117:THR:HG22	1:D:146:SER:HB2	1.99	0.44
1:D:124:ASP:O	1:D:128:GLN:HG3	2.18	0.44
1:D:114:CYS:O	1:D:144:ASN:HB2	2.17	0.44
1:D:214:PRO:HB2	1:D:259:ILE:HG22	2.00	0.44
1:C:138:ILE:HG21	1:C:147:PHE:CZ	2.52	0.44
1:A:181:ARG:HB3	1:A:181:ARG:HE	1.45	0.44
1:D:153:GLN:HB2	1:D:156:ARG:HG3	2.00	0.44
1:C:277:LEU:HD23	1:C:277:LEU:C	2.37	0.44
1:D:210:TYR:O	1:D:215:HIS:CE1	2.70	0.44
1:B:148:ASN:OD1	1:C:243:ARG:HG2	2.18	0.44
1:B:191:LEU:HD21	1:B:269:TYR:CZ	2.52	0.43
1:B:238:ARG:NH1	3:B:11:HOH:O	2.51	0.43
1:D:222:ASP:HA	1:D:225:LYS:HB3	2.00	0.43
1:A:112:GLN:CG	1:A:112:GLN:O	2.65	0.43
1:A:131:LEU:O	1:A:132:PRO:C	2.56	0.43
1:A:192:CYS:O	1:A:279:VAL:HA	2.18	0.43
1:D:210:TYR:HB2	1:D:283:PRO:HG2	2.01	0.43
1:C:132:PRO:O	1:C:136:PRO:HD3	2.18	0.43
1:B:316:CYS:O	1:B:320:ILE:HG12	2.18	0.43
1:B:218:ILE:HB	1:B:263:VAL:HG12	2.00	0.43
1:D:191:LEU:HA	1:D:191:LEU:HD12	1.82	0.43
1:D:250:ALA:HB1	1:D:261:ILE:HD13	1.99	0.43
1:B:320:ILE:H	1:B:320:ILE:HG12	1.57	0.43
1:C:210:TYR:HB2	1:C:283:PRO:HG3	2.00	0.43
1:D:131:LEU:HD22	1:D:131:LEU:N	2.34	0.43
1:D:256:THR:HG22	1:D:257:LEU:CD2	2.41	0.43
1:A:266:ASP:OD2	1:A:266:ASP:N	2.50	0.43
1:C:194:LEU:CD2	1:C:260:ILE:HG13	2.49	0.43
1:C:153:GLN:HB3	1:C:156:ARG:HB2	2.01	0.43
1:C:322:LYS:HE2	1:C:322:LYS:HB3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD11	1:D:268:ALA:HB1	2.00	0.43
1:C:271:VAL:HG13	1:C:275:TYR:CE2	2.54	0.43
1:C:194:LEU:HB2	1:C:278:VAL:CG2	2.48	0.43
1:D:172:ARG:HG2	1:D:172:ARG:O	2.16	0.43
1:B:230:GLN:HA	1:B:230:GLN:NE2	2.34	0.43
1:B:132:PRO:HA	1:C:252:ALA:CB	2.49	0.43
1:B:242:LEU:HD12	1:B:243:ARG:H	1.84	0.43
1:A:282:LEU:C	1:A:284:PHE:H	2.22	0.43
1:C:161:LEU:HD21	1:C:169:ALA:HB2	1.99	0.43
1:C:263:VAL:HG23	1:C:268:ALA:HB2	2.00	0.43
1:D:192:CYS:SG	1:D:210:TYR:HE2	2.41	0.43
1:A:144:ASN:HD22	1:A:144:ASN:N	2.17	0.43
1:B:123:THR:HB	3:B:38:HOH:O	2.18	0.43
1:A:321:ALA:O	1:A:322:LYS:C	2.57	0.42
1:A:193:LEU:HA	1:A:278:VAL:O	2.19	0.42
1:A:242:LEU:HD12	1:A:243:ARG:N	2.34	0.42
1:D:286:PHE:O	1:D:288:PRO:HD3	2.18	0.42
1:B:217:MSE:HE3	1:B:220:ILE:HG21	2.01	0.42
1:D:192:CYS:HG	1:D:210:TYR:HE2	1.68	0.42
1:A:126:ALA:HB2	1:A:291:TYR:HE2	1.84	0.42
1:B:161:LEU:HD21	1:B:169:ALA:HB2	2.01	0.42
1:A:218:ILE:CD1	1:A:244:ALA:HB3	2.49	0.42
1:B:156:ARG:NH1	1:B:164:GLU:OE2	2.49	0.42
1:A:275:TYR:O	1:A:276:ASP:C	2.58	0.42
1:A:178:GLU:H	1:A:178:GLU:CD	2.22	0.42
1:B:194:LEU:HD23	1:B:194:LEU:N	2.33	0.42
1:C:181:ARG:CD	1:C:300:GLU:OE1	2.66	0.42
1:D:120:ILE:HD13	1:D:120:ILE:N	2.35	0.42
1:A:314:GLU:HA	1:A:317:SER:HB2	2.02	0.42
1:D:293:MSE:O	1:D:294:ILE:HD13	2.19	0.42
1:C:178:GLU:H	1:C:178:GLU:HG3	1.65	0.42
1:C:250:ALA:HB1	1:C:261:ILE:HD13	2.01	0.42
1:B:228:ILE:HG12	1:B:286:PHE:CE1	2.54	0.42
1:B:215:HIS:CE1	1:B:238:ARG:HB2	2.55	0.42
1:A:320:ILE:HG12	1:A:323:ARG:HH21	1.85	0.41
1:A:305:GLN:O	1:A:309:ARG:HG3	2.20	0.41
1:D:185:LEU:HD22	1:D:316:CYS:SG	2.60	0.41
1:A:247:LEU:HD21	1:A:271:VAL:HG11	2.02	0.41
1:A:142:ALA:O	1:A:145:VAL:HB	2.21	0.41
1:B:118:PHE:N	1:B:118:PHE:CD1	2.88	0.41
1:C:235:LYS:HE3	1:C:236:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:HIS:CD2	1:B:238:ARG:HD2	2.55	0.41
1:A:114:CYS:O	1:A:144:ASN:HB2	2.20	0.41
1:B:188:VAL:HG21	1:B:291:TYR:CD1	2.55	0.41
1:B:124:ASP:OD2	1:C:246:HIS:ND1	2.53	0.41
1:D:191:LEU:HB2	1:D:265:ALA:HA	2.02	0.41
1:C:205:MSE:O	1:C:283:PRO:HB3	2.20	0.41
1:D:131:LEU:HB2	1:D:132:PRO:HD3	2.02	0.41
1:B:151:PRO:HB3	3:B:25:HOH:O	2.20	0.41
1:B:266:ASP:HB3	1:B:323:ARG:NH1	2.34	0.41
1:D:230:GLN:NE2	1:D:233:ILE:HD13	2.36	0.41
1:A:123:THR:O	1:A:127:MSE:HB2	2.20	0.41
1:D:115:ASP:OD1	1:D:115:ASP:C	2.59	0.41
1:C:247:LEU:HD11	1:C:271:VAL:CG1	2.36	0.41
1:A:320:ILE:O	1:A:321:ALA:C	2.59	0.41
1:B:265:ALA:O	1:B:268:ALA:HB3	2.19	0.41
1:D:282:LEU:HD22	1:D:282:LEU:HA	1.82	0.41
1:D:257:LEU:N	1:D:257:LEU:CD2	2.83	0.41
1:D:230:GLN:HA	1:D:233:ILE:HD13	2.03	0.41
1:C:135:LEU:N	1:C:136:PRO:CD	2.84	0.41
1:B:209:ASP:O	1:B:213:HIS:HD2	2.04	0.41
1:A:217:MSE:HE2	3:A:60:HOH:O	2.21	0.41
1:B:215:HIS:CG	1:B:238:ARG:HD2	2.56	0.41
1:C:230:GLN:O	1:C:233:ILE:HB	2.21	0.41
1:C:168:LEU:HD12	1:C:294:ILE:O	2.21	0.41
1:C:315:GLU:OE1	1:C:315:GLU:HA	2.21	0.41
1:C:270:LEU:HD22	1:C:270:LEU:O	2.21	0.41
1:B:128:GLN:HG2	1:C:248:GLU:HG3	2.03	0.41
1:B:137:ARG:HG3	1:B:137:ARG:NH1	2.35	0.41
1:D:218:ILE:HD13	1:D:218:ILE:HA	1.80	0.40
1:A:193:LEU:O	1:A:194:LEU:HD23	2.21	0.40
1:C:156:ARG:HD2	1:C:159:ASP:HB2	2.04	0.40
1:B:323:ARG:CG	1:B:323:ARG:HH11	2.34	0.40
1:C:246:HIS:CD2	1:C:246:HIS:N	2.88	0.40
1:B:271:VAL:HG22	1:B:275:TYR:HE2	1.87	0.40
1:B:240:MSE:O	1:C:146:SER:OG	2.39	0.40
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.88	0.40
1:C:192:CYS:CB	1:C:205:MSE:HE1	2.51	0.40
1:D:120:ILE:HD11	1:D:308:LEU:HD11	2.03	0.40
1:B:167:ASP:CG	1:B:305:GLN:NE2	2.75	0.40
1:A:127:MSE:HE1	1:A:149:PHE:CD2	2.56	0.40
1:C:230:GLN:NE2	1:C:233:ILE:HD13	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:VAL:HG12	1:C:282:LEU:HD11	2.03	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	209/241 (87%)	192 (92%)	14 (7%)	3 (1%)	14	35
1	B	214/241 (89%)	191 (89%)	19 (9%)	4 (2%)	10	25
1	C	209/241 (87%)	191 (91%)	16 (8%)	2 (1%)	19	45
1	D	210/241 (87%)	195 (93%)	14 (7%)	1 (0%)	34	63
All	All	842/964 (87%)	769 (91%)	63 (8%)	10 (1%)	16	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ALA
1	B	257	LEU
1	C	236	PRO
1	A	276	ASP
1	B	276	ASP
1	D	221	SER
1	C	322	LYS
1	A	322	LYS
1	B	130	ILE
1	B	258	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	186/206 (90%)	152 (82%)	34 (18%)	2 5
1	B	189/206 (92%)	157 (83%)	32 (17%)	2 6
1	C	187/206 (91%)	160 (86%)	27 (14%)	4 10
1	D	184/206 (89%)	158 (86%)	26 (14%)	4 10
All	All	746/824 (90%)	627 (84%)	119 (16%)	3 8

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	113	GLN
1	A	117	THR
1	A	122	THR
1	A	137	ARG
1	A	141	GLU
1	A	145	VAL
1	A	150	LEU
1	A	152	LEU
1	A	154	HIS
1	A	155	ASP
1	A	164	GLU
1	A	187	ARG
1	A	193	LEU
1	A	206	SER
1	A	211	LEU
1	A	212	SER
1	A	229	GLU
1	A	232	LEU
1	A	237	GLN
1	A	247	LEU
1	A	248	GLU
1	A	266	ASP
1	A	273	GLU

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Mol	Chain	Res	Type
1	A	276	ASP
1	A	277	LEU
1	A	290	ASP
1	A	291	TYR
1	A	292	SER
1	A	298	ARG
1	A	308	LEU
1	A	311	VAL
1	A	317	SER
1	A	318	ARG
1	B	117	THR
1	B	122	THR
1	B	141	GLU
1	B	150	LEU
1	B	152	LEU
1	B	154	HIS
1	B	156	ARG
1	B	172	ARG
1	B	177	VAL
1	B	187	ARG
1	B	188	VAL
1	B	190	VAL
1	B	191	LEU
1	B	193	LEU
1	B	196	LYS
1	B	205	MSE
1	B	211	LEU
1	B	227	LEU
1	B	229	GLU
1	B	241	VAL
1	B	257	LEU
1	B	266	ASP
1	B	270	LEU
1	B	271	VAL
1	B	276	ASP
1	B	277	LEU
1	B	291	TYR
1	B	298	ARG
1	B	308	LEU
1	B	318	ARG
1	B	320	ILE
1	B	323	ARG

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Mol	Chain	Res	Type
1	C	117	THR
1	C	122	THR
1	C	137	ARG
1	C	153	GLN
1	C	154	HIS
1	C	155	ASP
1	C	156	ARG
1	C	190	VAL
1	C	191	LEU
1	C	193	LEU
1	C	197	GLN
1	C	203	GLN
1	C	204	GLU
1	C	211	LEU
1	C	227	LEU
1	C	229	GLU
1	C	233	ILE
1	C	247	LEU
1	C	266	ASP
1	C	273	GLU
1	C	274	ARG
1	C	277	LEU
1	C	285	GLN
1	C	291	TYR
1	C	298	ARG
1	C	308	LEU
1	C	320	ILE
1	D	112	GLN
1	D	117	THR
1	D	122	THR
1	D	137	ARG
1	D	155	ASP
1	D	156	ARG
1	D	191	LEU
1	D	193	LEU
1	D	203	GLN
1	D	211	LEU
1	D	222	ASP
1	D	227	LEU
1	D	248	GLU
1	D	253	ILE
1	D	257	LEU

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Mol	Chain	Res	Type
1	D	270	LEU
1	D	271	VAL
1	D	273	GLU
1	D	277	LEU
1	D	280	LYS
1	D	282	LEU
1	D	285	GLN
1	D	291	TYR
1	D	298	ARG
1	D	308	LEU
1	D	320	ILE

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	128	GLN
1	A	144	ASN
1	A	213	HIS
1	A	230	GLN
1	A	246	HIS
1	B	128	GLN
1	B	213	HIS
1	B	230	GLN
1	B	246	HIS
1	B	305	GLN
1	C	113	GLN
1	C	153	GLN
1	C	215	HIS
1	C	230	GLN
1	C	246	HIS
1	D	144	ASN
1	D	160	GLN
1	D	215	HIS
1	D	230	GLN
1	D	246	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	SO4	D	1	-	4,4,4	0.09	0	6,6,6	0.26	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
2	SO4	D	1	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	208/241 (86%)	-0.45	0	100	100	27, 38, 57, 66	0
1	B	210/241 (87%)	-0.44	1 (0%)	91	93	26, 38, 53, 78	0
1	C	208/241 (86%)	-0.21	1 (0%)	91	93	32, 45, 58, 69	0
1	D	207/241 (85%)	-0.22	1 (0%)	91	93	29, 45, 60, 71	0
All	All	833/964 (86%)	-0.33	3 (0%)	93	94	26, 41, 58, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	GLU	2.7
1	D	273	GLU	2.5
1	B	113	GLN	2.5

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
2	SO4	D	1	5/5	0.97	0.12	-1.20	44,49,53,58	0

6.5 Other polymers (i)

There are no such residues in this entry.