Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U5W
Title	:	Crystal structure of hypothetical protein yjjX from Escherichia coli
Authors	:	Zheng, J.; Singh, V.K.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2004-07-28
Resolution	:	2.30 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:

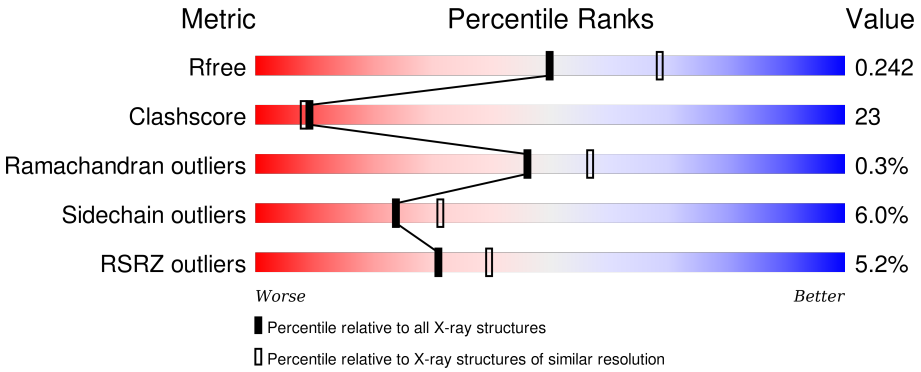
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	184	6% 54% 30% • 12%
1	B	184	2% 64% 27% • 7%
1	C	184	7% 61% 30% • 5%
1	D	184	3% 67% 26% • 7%
1	E	184	7% 56% 34% • 7%

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Mol	Chain	Length	Quality of chain
1	F	184	2% 61% 29% 7%
1	G	184	10% 51% 36% 9%
1	H	184	2% 51% 37% 5% 8%

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	SO4	E	4408	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11017 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 Hypothetical UPF0244 protein yjjX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1219	768	218	229	4			
1	B	172	Total	C	N	O	S	0	0	0
			1297	817	232	244	4			
1	C	174	Total	C	N	O	S	0	0	0
			1309	825	234	246	4			
1	D	172	Total	C	N	O	S	0	0	0
			1297	817	232	244	4			
1	E	172	Total	C	N	O	S	0	0	0
			1297	817	232	244	4			
1	F	172	Total	C	N	O	S	0	0	0
			1293	813	232	244	4			
1	G	168	Total	C	N	O	S	0	0	0
			1265	800	225	236	4			
1	H	170	Total	C	N	O	S	0	0	0
			1283	808	230	241	4			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P39411
A	2	LEU	-	cloning artifact	UNP P39411
A	3	ILE	-	cloning artifact	UNP P39411
A	174	SER	-	cloning artifact	UNP P39411
A	175	GLY	-	cloning artifact	UNP P39411
A	176	ARG	-	cloning artifact	UNP P39411
A	177	VAL	-	cloning artifact	UNP P39411
A	178	GLU	-	cloning artifact	UNP P39411
A	179	HIS	-	EXPRESSION TAG	UNP P39411
A	180	HIS	-	EXPRESSION TAG	UNP P39411
A	181	HIS	-	EXPRESSION TAG	UNP P39411
A	182	HIS	-	EXPRESSION TAG	UNP P39411
A	183	HIS	-	EXPRESSION TAG	UNP P39411

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Chain	Residue	Modelled	Actual	Comment	Reference
A	184	HIS	-	EXPRESSION TAG	UNP P39411
B	1	MET	-	cloning artifact	UNP P39411
B	2	LEU	-	cloning artifact	UNP P39411
B	3	ILE	-	cloning artifact	UNP P39411
B	174	SER	-	cloning artifact	UNP P39411
B	175	GLY	-	cloning artifact	UNP P39411
B	176	ARG	-	cloning artifact	UNP P39411
B	177	VAL	-	cloning artifact	UNP P39411
B	178	GLU	-	cloning artifact	UNP P39411
B	179	HIS	-	EXPRESSION TAG	UNP P39411
B	180	HIS	-	EXPRESSION TAG	UNP P39411
B	181	HIS	-	EXPRESSION TAG	UNP P39411
B	182	HIS	-	EXPRESSION TAG	UNP P39411
B	183	HIS	-	EXPRESSION TAG	UNP P39411
B	184	HIS	-	EXPRESSION TAG	UNP P39411
C	1	MET	-	cloning artifact	UNP P39411
C	2	LEU	-	cloning artifact	UNP P39411
C	3	ILE	-	cloning artifact	UNP P39411
C	174	SER	-	cloning artifact	UNP P39411
C	175	GLY	-	cloning artifact	UNP P39411
C	176	ARG	-	cloning artifact	UNP P39411
C	177	VAL	-	cloning artifact	UNP P39411
C	178	GLU	-	cloning artifact	UNP P39411
C	179	HIS	-	EXPRESSION TAG	UNP P39411
C	180	HIS	-	EXPRESSION TAG	UNP P39411
C	181	HIS	-	EXPRESSION TAG	UNP P39411
C	182	HIS	-	EXPRESSION TAG	UNP P39411
C	183	HIS	-	EXPRESSION TAG	UNP P39411
C	184	HIS	-	EXPRESSION TAG	UNP P39411
D	1	MET	-	cloning artifact	UNP P39411
D	2	LEU	-	cloning artifact	UNP P39411
D	3	ILE	-	cloning artifact	UNP P39411
D	174	SER	-	cloning artifact	UNP P39411
D	175	GLY	-	cloning artifact	UNP P39411
D	176	ARG	-	cloning artifact	UNP P39411
D	177	VAL	-	cloning artifact	UNP P39411
D	178	GLU	-	cloning artifact	UNP P39411
D	179	HIS	-	EXPRESSION TAG	UNP P39411
D	180	HIS	-	EXPRESSION TAG	UNP P39411
D	181	HIS	-	EXPRESSION TAG	UNP P39411
D	182	HIS	-	EXPRESSION TAG	UNP P39411
D	183	HIS	-	EXPRESSION TAG	UNP P39411

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Chain	Residue	Modelled	Actual	Comment	Reference
D	184	HIS	-	EXPRESSION TAG	UNP P39411
E	1	MET	-	cloning artifact	UNP P39411
E	2	LEU	-	cloning artifact	UNP P39411
E	3	ILE	-	cloning artifact	UNP P39411
E	174	SER	-	cloning artifact	UNP P39411
E	175	GLY	-	cloning artifact	UNP P39411
E	176	ARG	-	cloning artifact	UNP P39411
E	177	VAL	-	cloning artifact	UNP P39411
E	178	GLU	-	cloning artifact	UNP P39411
E	179	HIS	-	EXPRESSION TAG	UNP P39411
E	180	HIS	-	EXPRESSION TAG	UNP P39411
E	181	HIS	-	EXPRESSION TAG	UNP P39411
E	182	HIS	-	EXPRESSION TAG	UNP P39411
E	183	HIS	-	EXPRESSION TAG	UNP P39411
E	184	HIS	-	EXPRESSION TAG	UNP P39411
F	1	MET	-	cloning artifact	UNP P39411
F	2	LEU	-	cloning artifact	UNP P39411
F	3	ILE	-	cloning artifact	UNP P39411
F	174	SER	-	cloning artifact	UNP P39411
F	175	GLY	-	cloning artifact	UNP P39411
F	176	ARG	-	cloning artifact	UNP P39411
F	177	VAL	-	cloning artifact	UNP P39411
F	178	GLU	-	cloning artifact	UNP P39411
F	179	HIS	-	EXPRESSION TAG	UNP P39411
F	180	HIS	-	EXPRESSION TAG	UNP P39411
F	181	HIS	-	EXPRESSION TAG	UNP P39411
F	182	HIS	-	EXPRESSION TAG	UNP P39411
F	183	HIS	-	EXPRESSION TAG	UNP P39411
F	184	HIS	-	EXPRESSION TAG	UNP P39411
G	1	MET	-	cloning artifact	UNP P39411
G	2	LEU	-	cloning artifact	UNP P39411
G	3	ILE	-	cloning artifact	UNP P39411
G	174	SER	-	cloning artifact	UNP P39411
G	175	GLY	-	cloning artifact	UNP P39411
G	176	ARG	-	cloning artifact	UNP P39411
G	177	VAL	-	cloning artifact	UNP P39411
G	178	GLU	-	cloning artifact	UNP P39411
G	179	HIS	-	EXPRESSION TAG	UNP P39411
G	180	HIS	-	EXPRESSION TAG	UNP P39411
G	181	HIS	-	EXPRESSION TAG	UNP P39411
G	182	HIS	-	EXPRESSION TAG	UNP P39411
G	183	HIS	-	EXPRESSION TAG	UNP P39411

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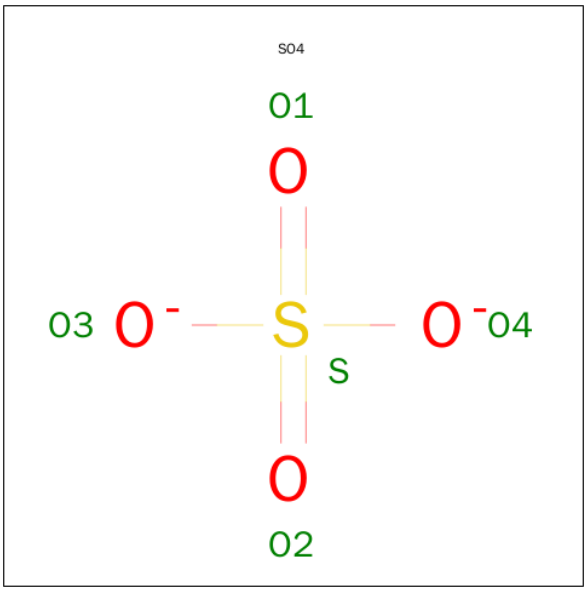
Chain	Residue	Modelled	Actual	Comment	Reference
G	184	HIS	-	EXPRESSION TAG	UNP P39411
H	1	MET	-	cloning artifact	UNP P39411
H	2	LEU	-	cloning artifact	UNP P39411
H	3	ILE	-	cloning artifact	UNP P39411
H	174	SER	-	cloning artifact	UNP P39411
H	175	GLY	-	cloning artifact	UNP P39411
H	176	ARG	-	cloning artifact	UNP P39411
H	177	VAL	-	cloning artifact	UNP P39411
H	178	GLU	-	cloning artifact	UNP P39411
H	179	HIS	-	EXPRESSION TAG	UNP P39411
H	180	HIS	-	EXPRESSION TAG	UNP P39411
H	181	HIS	-	EXPRESSION TAG	UNP P39411
H	182	HIS	-	EXPRESSION TAG	UNP P39411
H	183	HIS	-	EXPRESSION TAG	UNP P39411
H	184	HIS	-	EXPRESSION TAG	UNP P39411

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

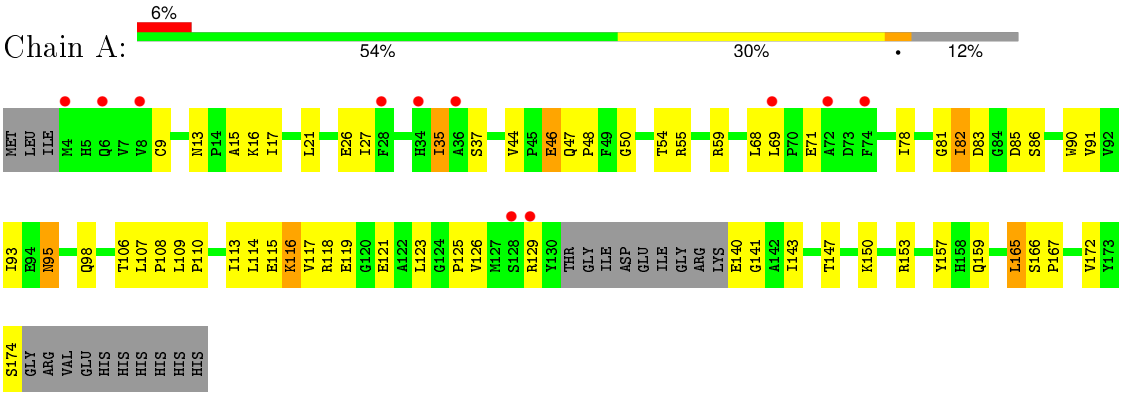
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	106	Total O 106 106	0	0
3	C	92	Total O 92 92	0	0
3	D	110	Total O 110 110	0	0
3	E	68	Total O 68 68	0	0
3	F	92	Total O 92 92	0	0
3	G	69	Total O 69 69	0	0
3	H	72	Total O 72 72	0	0

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.

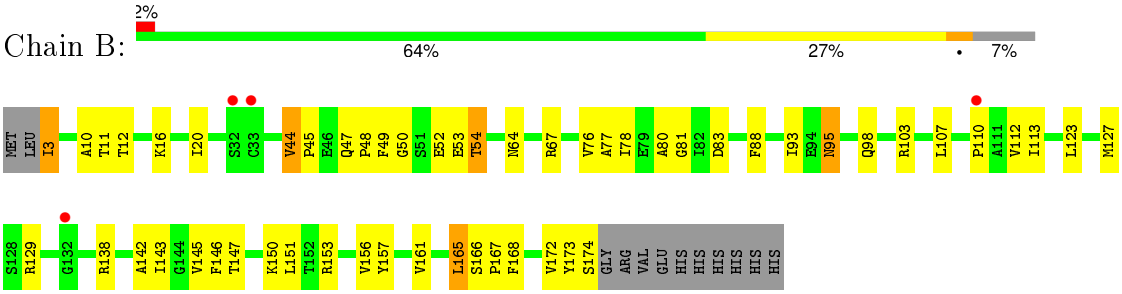
- Molecule 1: Hypothetical UPF0244 protein yjjX

Chain A:



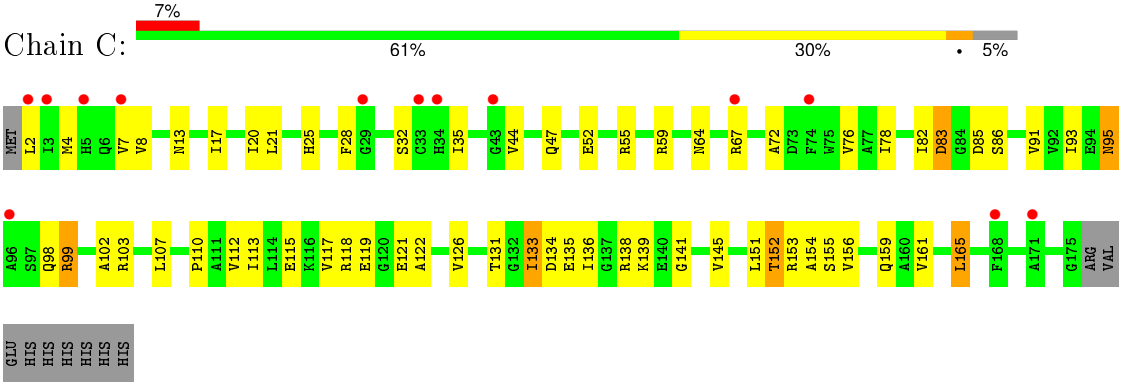
- Molecule 1: Hypothetical UPF0244 protein yjjX

Chain B:



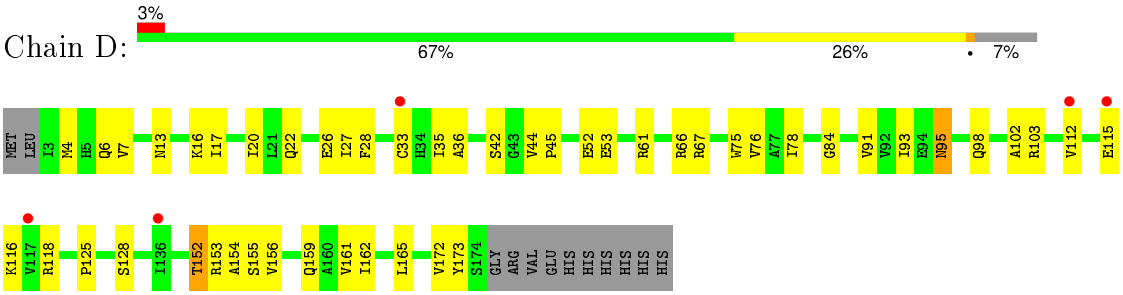
- Molecule 1: Hypothetical UPF0244 protein yjjX

Chain C:



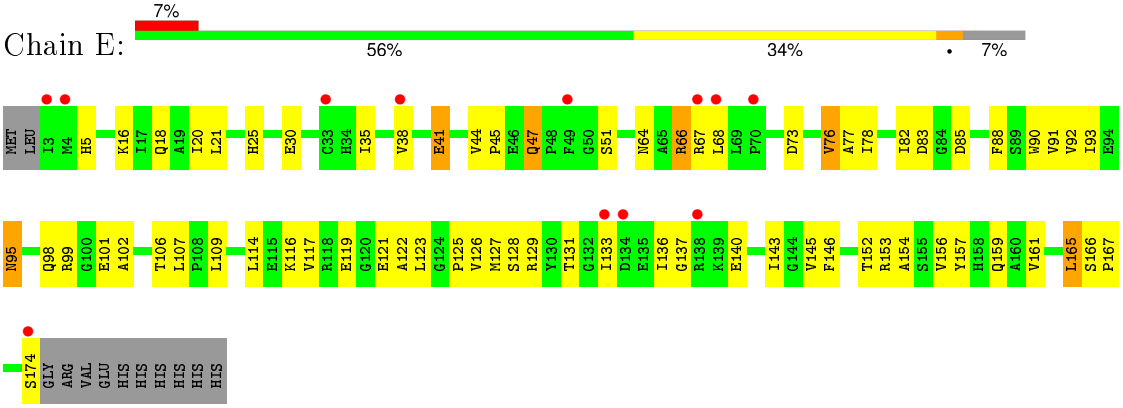
- Molecule 1: Hypothetical UPF0244 protein yjjX

Chain D:



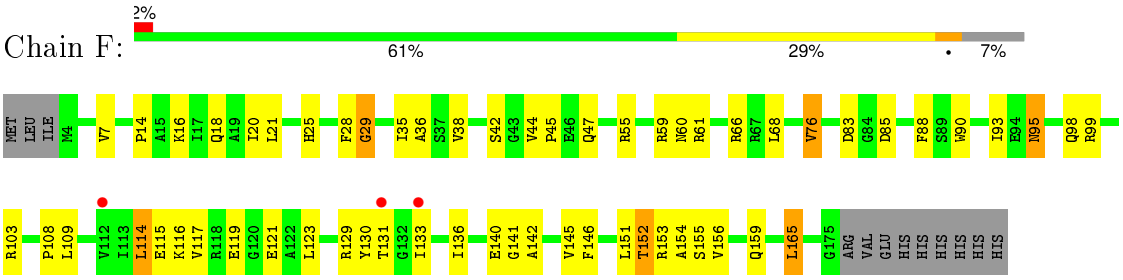
• Molecule 1: Hypothetical UPF0244 protein yjjX

Chain E:



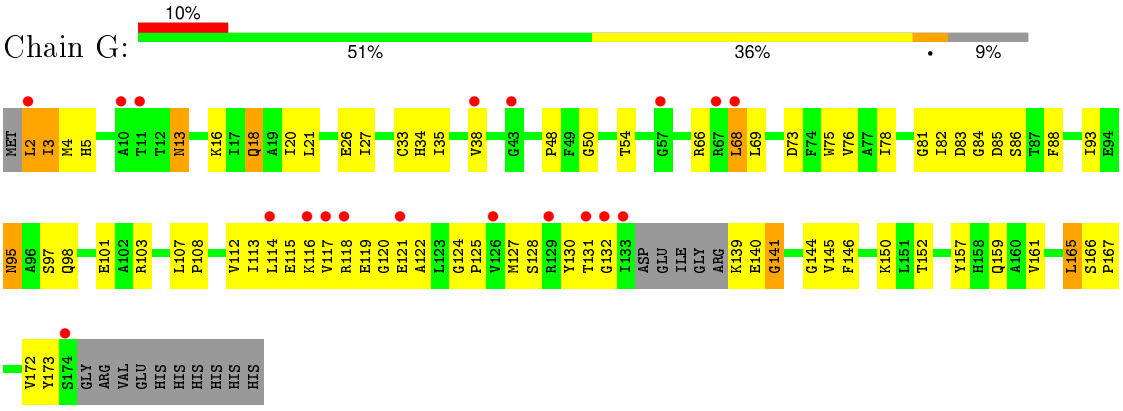
• Molecule 1: Hypothetical UPF0244 protein yjjX

Chain F:



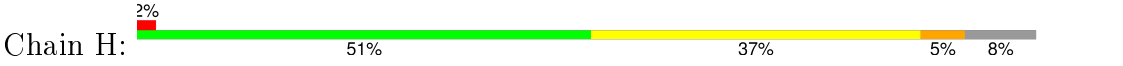
• Molecule 1: Hypothetical UPF0244 protein yjjX

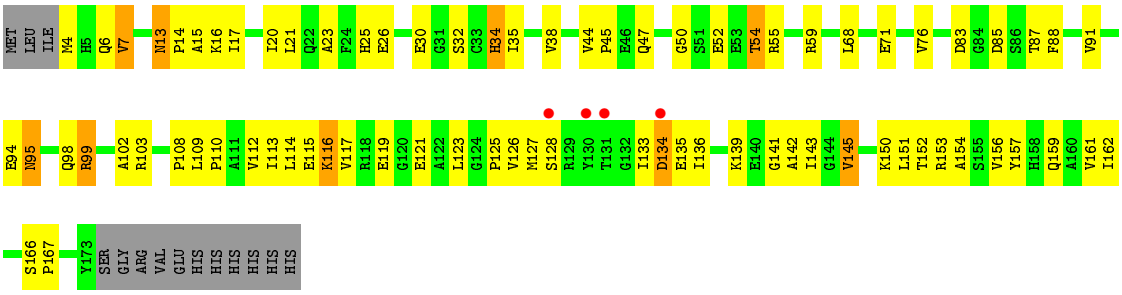
Chain G:



• Molecule 1: Hypothetical UPF0244 protein yjjX

Chain H:




MET
LEU
ILE
M4
H5
Q6
V7
N13
P14
A15
K16
I17
I20
L21
Q22
A23
F24
H25
E26
E30
G31
S32
C33
H34
I35
V38
V44
P45
E46
Q47
G50
S51
E52
E53
T54
R55
R59
L68
E71
V76
D83
G84
D85
S86
T87
F88
V91
E94
N95
Q98
R99
A102
R103
P108
L109
P110
A111
V112
I113
L114
E115
K116
V117
R118
E119
G120
E121
A122
L123
G124
P125
V126
M127
S128
R129
Y130
T131
G132
I133
D134
E135
I136
K139
E140
G141
A142
I143
G144
V145
K150
L151
T152
R153
A154
S155
V156
Y157
H158
Q159
A160
V161
I162
S166
P167
Y173
SER
GLY
ARG
VAL
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.00Å 129.34Å 85.38Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 29.27 – 2.23	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 91.0 (29.27-2.23)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.255 0.244 , 0.242	Depositor DCC
R_{free} test set	3194 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 17.7	EDS
Estimated twinning fraction	0.120 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 68100 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11017	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.37	0/1243	0.66	1/1688 (0.1%)
1	B	0.35	0/1323	0.59	0/1797
1	C	0.35	0/1335	0.60	0/1813
1	D	0.35	0/1323	0.59	0/1797
1	E	0.34	0/1323	0.56	0/1797
1	F	0.34	0/1319	0.58	0/1791
1	G	0.34	0/1290	0.57	0/1752
1	H	0.34	0/1309	0.56	0/1778
All	All	0.35	0/10465	0.59	1/14213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	PRO	N-CA-CB	5.41	109.79	103.30

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	1219	0	1196	60	0
1	B	1297	0	1285	51	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1309	0	1299	66	0
1	D	1297	0	1285	48	0
1	E	1297	0	1285	69	3
1	F	1293	0	1277	62	0
1	G	1265	0	1258	74	0
1	H	1283	0	1269	68	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	73	0	0	6	0
3	B	106	0	0	3	0
3	C	92	0	0	4	0
3	D	110	0	0	3	3
3	E	68	0	0	6	0
3	F	92	0	0	6	0
3	G	69	0	0	3	1
3	H	72	0	0	8	0
All	All	11017	0	10154	472	4

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 23.

All (472) 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:D:152:THR:HG22	1:D:155:SER:H	1.29	0.96
1:B:44:VAL:HG22	1:B:45:PRO:HD2	1.46	0.96
1:G:3:ILE:H	1:G:3:ILE:HD13	1.31	0.94
1:F:152:THR:HG22	1:F:155:SER:H	1.31	0.93
1:A:95:ASN:HD21	1:A:98:GLN:H	1.09	0.93
1:F:95:ASN:ND2	1:F:98:GLN:H	1.67	0.92
1:H:152:THR:HG22	1:H:154:ALA:H	1.35	0.91
1:E:95:ASN:HD21	1:E:98:GLN:H	1.13	0.90
1:E:95:ASN:ND2	1:E:98:GLN:H	1.69	0.89
1:B:95:ASN:ND2	1:B:98:GLN:H	1.70	0.88
1:B:50:GLY:O	1:B:54:THR:HG23	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ASN:ND2	1:G:98:GLN:H	1.71	0.87
1:B:12:THR:HG22	1:B:138:ARG:HH12	1.38	0.87
1:D:95:ASN:ND2	1:D:98:GLN:H	1.73	0.86
1:C:133:ILE:HD11	1:C:139:LYS:HD2	1.54	0.86
1:F:116:LYS:HZ3	1:F:129:ARG:HH21	1.22	0.85
1:H:95:ASN:ND2	1:H:98:GLN:H	1.73	0.85
1:C:131:THR:OG1	1:C:133:ILE:HG22	1.75	0.84
1:C:135:GLU:HG2	1:C:138:ARG:HD3	1.59	0.84
1:F:95:ASN:HD21	1:F:98:GLN:H	1.21	0.84
1:A:13:ASN:HD21	1:A:15:ALA:HB3	1.44	0.82
1:A:50:GLY:O	1:A:54:THR:HG23	1.80	0.81
1:E:51:SER:HB2	1:E:90:TRP:HE1	1.44	0.81
1:H:21:LEU:HD13	1:H:35:ILE:HD13	1.64	0.80
1:B:95:ASN:HD21	1:B:98:GLN:H	1.27	0.80
1:F:116:LYS:NZ	1:F:129:ARG:HH21	1.80	0.80
1:F:131:THR:OG1	1:F:133:ILE:HG22	1.82	0.80
1:G:95:ASN:HD21	1:G:98:GLN:H	1.28	0.79
1:A:93:ILE:HD13	1:A:165:LEU:HD13	1.64	0.79
1:F:93:ILE:HD13	1:F:165:LEU:HD13	1.64	0.79
1:C:152:THR:HG22	1:C:155:SER:H	1.48	0.78
1:D:44:VAL:HG22	1:D:45:PRO:HD2	1.66	0.78
1:H:50:GLY:O	1:H:54:THR:HG22	1.83	0.78
1:A:13:ASN:ND2	1:A:16:LYS:H	1.83	0.77
1:A:95:ASN:ND2	1:A:98:GLN:H	1.80	0.77
1:A:13:ASN:HD22	1:A:16:LYS:H	1.30	0.77
1:G:93:ILE:HD13	1:G:165:LEU:HD13	1.68	0.76
1:E:35:ILE:HB	1:G:35:ILE:HB	1.69	0.74
1:H:83:ASP:HB2	1:H:88:PHE:HE2	1.52	0.74
1:A:27:ILE:HD12	1:A:165:LEU:HD23	1.70	0.74
1:G:139:LYS:HG2	1:G:141:GLY:H	1.52	0.74
1:B:12:THR:HG22	1:B:138:ARG:NH1	2.03	0.73
1:E:152:THR:HG22	1:E:154:ALA:H	1.53	0.73
1:F:38:VAL:HG21	1:F:68:LEU:HD13	1.70	0.73
1:E:68:LEU:HD13	1:G:2:LEU:HD23	1.72	0.72
1:E:85:ASP:HA	1:E:114:LEU:HD21	1.72	0.71
1:A:143:ILE:HD12	1:A:153:ARG:HD2	1.70	0.71
1:G:26:GLU:O	1:H:150:LYS:HE3	1.90	0.71
1:C:95:ASN:ND2	1:C:98:GLN:H	1.87	0.71
1:H:44:VAL:HG13	1:H:45:PRO:HD2	1.71	0.70
1:H:95:ASN:HD21	1:H:98:GLN:H	1.35	0.70
1:H:4:MET:HA	3:H:4438:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:H	1:A:35:ILE:HD13	1.56	0.70
1:C:159:GLN:HE22	1:D:156:VAL:HA	1.55	0.70
1:E:91:VAL:HG12	1:E:102:ALA:O	1.92	0.70
1:G:4:MET:HB2	1:G:33:CYS:HA	1.74	0.69
1:F:83:ASP:HB2	1:F:88:PHE:CE2	2.28	0.69
1:F:133:ILE:HG23	1:F:136:ILE:HB	1.74	0.68
1:F:16:LYS:O	1:F:20:ILE:HG12	1.93	0.68
1:A:85:ASP:HB2	3:A:4455:HOH:O	1.91	0.68
1:H:16:LYS:O	1:H:20:ILE:HG12	1.93	0.68
1:E:47:GLN:HG3	1:E:122:ALA:HA	1.74	0.68
1:D:35:ILE:HG12	3:D:4482:HOH:O	1.94	0.68
1:F:152:THR:CG2	1:F:155:SER:H	2.03	0.68
1:C:55:ARG:HD3	1:C:59:ARG:CZ	2.24	0.68
1:G:50:GLY:O	1:G:54:THR:HG23	1.93	0.67
1:H:152:THR:HG22	1:H:154:ALA:N	2.08	0.67
1:G:3:ILE:H	1:G:3:ILE:CD1	2.06	0.67
1:C:115:GLU:O	1:C:119:GLU:HG2	1.94	0.67
1:F:116:LYS:HE2	1:F:121:GLU:OE2	1.95	0.67
1:C:17:ILE:HG23	1:C:35:ILE:HD13	1.77	0.67
1:A:82:ILE:H	1:A:82:ILE:HD13	1.58	0.66
1:D:44:VAL:CG2	1:D:45:PRO:HD2	2.25	0.66
1:B:127:MET:HE1	1:B:145:VAL:HG21	1.78	0.66
1:E:107:LEU:HD22	1:E:143:ILE:HD13	1.77	0.66
1:G:38:VAL:HG21	1:G:68:LEU:HD22	1.77	0.66
1:F:85:ASP:HA	1:F:114:LEU:HD21	1.77	0.66
1:E:20:ILE:HD13	1:E:161:VAL:HG21	1.78	0.65
1:G:5:HIS:HB3	1:G:73:ASP:OD1	1.96	0.65
1:A:95:ASN:HD21	1:A:98:GLN:N	1.90	0.65
1:F:47:GLN:HE21	1:F:123:LEU:H	1.44	0.65
1:G:116:LYS:O	1:G:119:GLU:HG2	1.97	0.65
1:E:66:ARG:HD2	3:E:4416:HOH:O	1.96	0.65
1:H:47:GLN:HE21	1:H:123:LEU:H	1.44	0.65
1:E:16:LYS:O	1:E:20:ILE:HG12	1.97	0.65
1:F:83:ASP:HB2	1:F:88:PHE:HE2	1.61	0.65
1:B:52:GLU:HB2	1:D:52:GLU:HB2	1.80	0.64
1:B:110:PRO:HG2	1:B:113:ILE:HD13	1.80	0.64
1:F:115:GLU:O	1:F:119:GLU:HG2	1.98	0.64
1:G:16:LYS:O	1:G:20:ILE:HG12	1.98	0.63
1:A:93:ILE:CD1	1:A:165:LEU:HD13	2.27	0.63
1:H:13:ASN:HD22	1:H:13:ASN:C	2.02	0.63
1:B:107:LEU:HD22	1:B:143:ILE:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LYS:O	1:E:119:GLU:HG2	1.99	0.63
1:G:127:MET:CE	1:G:145:VAL:HG21	2.29	0.63
1:G:85:ASP:HA	1:G:114:LEU:HD21	1.79	0.63
1:B:3:ILE:N	1:B:3:ILE:HD13	2.14	0.63
1:H:55:ARG:HD2	3:H:4461:HOH:O	1.98	0.62
1:B:93:ILE:CD1	1:B:165:LEU:HD22	2.29	0.62
1:B:127:MET:CE	1:B:145:VAL:HG21	2.30	0.62
1:D:95:ASN:HD21	1:D:98:GLN:H	1.45	0.61
1:C:136:ILE:HG12	1:C:141:GLY:HA2	1.83	0.61
1:C:20:ILE:HD13	1:C:161:VAL:HG21	1.82	0.61
1:H:136:ILE:HG12	1:H:141:GLY:HA2	1.83	0.61
1:D:152:THR:HG22	1:D:155:SER:N	2.09	0.61
1:F:140:GLU:HA	3:F:4476:HOH:O	1.99	0.61
1:C:110:PRO:HD3	1:D:173:TYR:CZ	2.36	0.61
1:E:44:VAL:HB	1:E:45:PRO:HD2	1.83	0.61
1:D:152:THR:HG23	1:D:154:ALA:H	1.65	0.61
1:F:95:ASN:HD21	1:F:98:GLN:N	1.94	0.61
1:E:152:THR:HG22	1:E:153:ARG:N	2.16	0.61
1:C:133:ILE:HD11	1:C:139:LYS:CD	2.27	0.60
1:C:152:THR:HG23	3:C:4426:HOH:O	2.01	0.60
1:F:47:GLN:NE2	1:F:123:LEU:H	1.98	0.60
1:G:120:GLY:O	1:G:121:GLU:HG3	2.01	0.60
1:A:109:LEU:HB2	1:A:114:LEU:HD21	1.82	0.60
1:C:55:ARG:HD2	3:C:4414:HOH:O	2.00	0.60
1:D:93:ILE:HD13	1:D:165:LEU:HD13	1.84	0.60
1:H:103:ARG:HH11	1:H:103:ARG:HG3	1.67	0.60
1:D:36:ALA:HB1	1:F:21:LEU:HD21	1.83	0.60
1:C:152:THR:CG2	1:C:154:ALA:H	2.15	0.60
1:F:44:VAL:HB	1:F:45:PRO:HD2	1.84	0.60
1:D:66:ARG:HG2	1:D:75:TRP:CD2	2.36	0.60
1:A:55:ARG:HD3	1:A:59:ARG:CZ	2.31	0.59
1:H:153:ARG:HG2	1:H:157:TYR:CE2	2.37	0.59
1:C:86:SER:HB2	1:C:107:LEU:O	2.03	0.59
1:D:20:ILE:HD12	1:D:76:VAL:HG21	1.85	0.59
1:E:121:GLU:HG2	3:E:4432:HOH:O	2.02	0.58
1:H:95:ASN:C	1:H:95:ASN:HD22	2.06	0.58
1:H:13:ASN:ND2	1:H:15:ALA:H	2.01	0.58
1:H:116:LYS:O	1:H:119:GLU:HG2	2.04	0.58
1:C:21:LEU:HB2	1:C:35:ILE:HD11	1.85	0.58
1:A:78:ILE:HG12	1:A:91:VAL:HG22	1.85	0.58
1:B:44:VAL:CG2	1:B:53:GLU:HG3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:VAL:HG12	1:D:102:ALA:O	2.04	0.58
1:A:98:GLN:HB2	3:A:4442:HOH:O	2.04	0.58
1:F:142:ALA:O	1:F:145:VAL:HG22	2.04	0.58
1:B:95:ASN:HD21	1:B:98:GLN:N	2.01	0.58
1:C:110:PRO:HG2	1:C:113:ILE:CG1	2.34	0.58
1:G:13:ASN:C	1:G:13:ASN:HD22	2.07	0.58
1:G:140:GLU:HB3	1:G:144:GLY:HA3	1.86	0.58
1:E:20:ILE:HD12	1:E:76:VAL:HG21	1.86	0.58
1:H:55:ARG:HD3	1:H:59:ARG:CZ	2.34	0.57
1:B:16:LYS:O	1:B:20:ILE:HG12	2.04	0.57
1:H:135:GLU:HG3	1:H:139:LYS:HE3	1.86	0.57
1:A:153:ARG:HG3	1:A:157:TYR:CZ	2.39	0.57
1:A:13:ASN:HD22	1:A:16:LYS:HG3	1.70	0.57
1:D:95:ASN:HD21	1:D:98:GLN:N	2.03	0.57
1:D:22:GLN:O	1:D:26:GLU:HG2	2.05	0.57
1:B:157:TYR:O	1:B:161:VAL:HG23	2.05	0.57
1:F:7:VAL:CG1	1:F:35:ILE:HD13	2.34	0.56
1:B:112:VAL:HG23	1:B:113:ILE:HD12	1.87	0.56
1:F:7:VAL:HG13	1:F:35:ILE:HD13	1.85	0.56
1:A:110:PRO:HB2	1:A:113:ILE:HG12	1.86	0.56
1:C:122:ALA:O	1:C:126:VAL:HG23	2.06	0.56
1:G:95:ASN:C	1:G:95:ASN:HD22	2.09	0.56
1:F:20:ILE:HD12	1:F:76:VAL:HG21	1.88	0.56
1:H:4:MET:HB2	1:H:32:SER:O	2.05	0.56
1:H:47:GLN:NE2	1:H:123:LEU:H	2.04	0.56
1:G:95:ASN:C	1:G:95:ASN:ND2	2.59	0.56
1:C:78:ILE:CD1	1:C:91:VAL:HB	2.36	0.56
1:C:133:ILE:HG23	1:C:136:ILE:HB	1.87	0.56
1:F:93:ILE:CD1	1:F:165:LEU:HD13	2.35	0.56
1:G:84:GLY:O	1:G:114:LEU:HD21	2.06	0.56
1:B:44:VAL:CG2	1:B:45:PRO:HD2	2.29	0.55
1:G:112:VAL:HG23	1:G:113:ILE:H	1.71	0.55
1:H:25:HIS:HB3	1:H:30:GLU:OE1	2.07	0.55
1:C:95:ASN:HD21	1:C:98:GLN:H	1.53	0.55
1:C:112:VAL:HG13	3:D:4422:HOH:O	2.05	0.55
1:G:166:SER:HB2	1:G:167:PRO:HD3	1.88	0.55
1:C:118:ARG:HD3	3:C:4470:HOH:O	2.06	0.55
1:C:76:VAL:HG12	1:C:93:ILE:HG23	1.88	0.55
1:G:2:LEU:O	1:G:2:LEU:HD12	2.06	0.55
1:E:64:ASN:ND2	1:E:67:ARG:HH21	2.04	0.55
1:B:172:VAL:C	1:B:174:SER:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ILE:HD11	1:G:78:ILE:HD11	1.89	0.55
1:C:152:THR:HG23	1:C:154:ALA:H	1.72	0.55
1:H:95:ASN:HD21	1:H:98:GLN:N	2.04	0.55
1:B:166:SER:HB2	1:B:167:PRO:HD3	1.89	0.55
1:E:131:THR:HB	1:E:133:ILE:HG22	1.89	0.54
1:H:95:ASN:ND2	1:H:95:ASN:C	2.59	0.54
1:D:44:VAL:CG2	1:D:53:GLU:HG3	2.37	0.54
1:A:116:LYS:HZ3	1:A:116:LYS:HB2	1.72	0.54
1:C:67:ARG:HH21	1:C:67:ARG:HG2	1.73	0.54
1:E:140:GLU:O	1:E:153:ARG:HG3	2.08	0.54
1:B:142:ALA:O	1:B:145:VAL:HG22	2.07	0.54
1:D:125:PRO:O	1:D:128:SER:HB3	2.07	0.54
1:C:21:LEU:HB2	1:C:35:ILE:CD1	2.37	0.53
1:D:95:ASN:ND2	1:D:98:GLN:N	2.51	0.53
1:E:109:LEU:HB2	1:E:114:LEU:HD13	1.90	0.53
1:D:66:ARG:HG2	1:D:75:TRP:CE2	2.44	0.53
1:H:91:VAL:HG12	1:H:102:ALA:O	2.09	0.53
1:G:115:GLU:HG3	1:G:116:LYS:N	2.23	0.53
1:B:20:ILE:HG21	1:B:76:VAL:HG21	1.91	0.53
3:A:4448:HOH:O	1:D:118:ARG:HD3	2.08	0.53
1:B:10:ALA:HB3	1:B:77:ALA:HB2	1.90	0.53
1:D:95:ASN:HD22	1:D:95:ASN:C	2.12	0.53
1:F:55:ARG:HD3	1:F:59:ARG:CZ	2.39	0.53
1:D:112:VAL:O	1:D:115:GLU:HG2	2.09	0.52
1:G:5:HIS:HD2	3:G:4401:HOH:O	1.92	0.52
1:E:117:VAL:CG1	1:E:126:VAL:HG11	2.38	0.52
1:A:116:LYS:HD2	1:A:121:GLU:OE1	2.09	0.52
1:A:115:GLU:O	1:A:119:GLU:HG3	2.10	0.52
1:G:152:THR:HG22	3:G:4413:HOH:O	2.08	0.52
1:G:95:ASN:HD21	1:G:98:GLN:N	2.04	0.52
1:H:13:ASN:HD22	1:H:15:ALA:H	1.58	0.52
1:E:129:ARG:NH2	3:E:4432:HOH:O	2.41	0.52
1:G:122:ALA:O	1:G:125:PRO:HG2	2.08	0.52
1:A:106:THR:HB	1:B:103:ARG:H	1.73	0.52
1:C:7:VAL:O	1:C:7:VAL:HG23	2.09	0.52
1:G:145:VAL:HG23	1:G:146:PHE:N	2.25	0.52
1:C:83:ASP:C	1:C:85:ASP:H	2.12	0.52
1:E:93:ILE:HD13	1:E:165:LEU:HD13	1.91	0.52
1:G:127:MET:HE1	1:G:145:VAL:HG21	1.92	0.52
1:E:119:GLU:O	1:E:119:GLU:HG3	2.09	0.52
1:A:143:ILE:O	1:A:147:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:HB2	1:F:114:LEU:HD13	1.91	0.52
1:E:64:ASN:HD22	1:E:67:ARG:HH21	1.57	0.52
1:E:82:ILE:HG22	1:E:83:ASP:N	2.25	0.52
1:E:159:GLN:HE22	1:F:156:VAL:HA	1.74	0.52
1:H:20:ILE:HD13	1:H:161:VAL:HG21	1.91	0.51
1:G:150:LYS:HE3	1:H:26:GLU:O	2.10	0.51
1:E:76:VAL:HB	1:E:93:ILE:HG12	1.91	0.51
1:A:68:LEU:C	1:A:69:LEU:HD12	2.31	0.51
1:E:18:GLN:OE1	1:G:18:GLN:HG3	2.10	0.51
1:H:7:VAL:HG13	1:H:35:ILE:HD12	1.92	0.51
1:B:83:ASP:HB2	1:B:88:PHE:CE2	2.45	0.51
1:A:123:LEU:HA	1:A:126:VAL:HG12	1.91	0.51
1:D:44:VAL:HG22	1:D:45:PRO:CD	2.39	0.51
1:A:107:LEU:HD12	1:A:108:PRO:HD2	1.91	0.51
1:B:49:PHE:CG	1:C:52:GLU:HG3	2.46	0.51
1:A:48:PRO:O	1:A:82:ILE:HD13	2.11	0.51
1:G:54:THR:HG21	1:G:81:GLY:HA3	1.92	0.51
1:E:95:ASN:HD21	1:E:98:GLN:N	1.94	0.51
1:H:23:ALA:HA	1:H:162:ILE:HD11	1.93	0.51
1:D:95:ASN:ND2	1:D:95:ASN:C	2.64	0.51
1:C:156:VAL:HA	1:D:159:GLN:HE22	1.76	0.51
1:A:114:LEU:O	1:A:117:VAL:HG22	2.11	0.51
1:H:30:GLU:O	1:H:30:GLU:HG3	2.11	0.51
1:C:47:GLN:NE2	1:C:82:ILE:HG12	2.26	0.51
1:A:13:ASN:ND2	1:A:16:LYS:HG3	2.26	0.51
1:D:118:ARG:HG3	1:D:118:ARG:HH11	1.75	0.51
1:B:49:PHE:CD1	1:C:52:GLU:HG3	2.45	0.51
1:A:95:ASN:HD22	1:A:95:ASN:C	2.14	0.51
1:G:114:LEU:O	1:G:117:VAL:HG22	2.09	0.51
1:E:67:ARG:NH1	1:E:67:ARG:HB2	2.26	0.51
1:H:34:HIS:CD2	1:H:34:HIS:C	2.85	0.51
1:C:110:PRO:HG2	1:C:113:ILE:HG12	1.93	0.50
1:B:142:ALA:HA	1:B:145:VAL:HG22	1.92	0.50
1:A:172:VAL:C	1:A:174:SER:H	2.13	0.50
1:B:64:ASN:HD22	1:B:67:ARG:HH11	1.58	0.50
1:A:140:GLU:HG3	1:A:141:GLY:N	2.25	0.50
1:A:13:ASN:O	1:A:17:ILE:HG13	2.11	0.50
1:C:95:ASN:HD21	1:C:98:GLN:N	2.08	0.50
1:F:152:THR:HG22	1:F:155:SER:N	2.13	0.50
1:H:44:VAL:HG13	1:H:45:PRO:CD	2.42	0.50
1:H:159:GLN:NE2	3:H:4413:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ILE:HG12	1:F:141:GLY:HA2	1.94	0.50
1:C:152:THR:HG22	1:C:154:ALA:N	2.26	0.50
1:C:117:VAL:HA	1:C:121:GLU:O	2.11	0.50
1:H:125:PRO:HA	1:H:128:SER:OG	2.12	0.50
1:E:82:ILE:CG2	1:E:83:ASP:N	2.75	0.50
1:E:156:VAL:HG23	1:E:157:TYR:N	2.26	0.50
3:G:4414:HOH:O	1:H:108:PRO:HG3	2.11	0.49
1:H:133:ILE:O	1:H:133:ILE:HG23	2.12	0.49
1:H:153:ARG:NH1	3:H:4439:HOH:O	2.44	0.49
1:C:52:GLU:H	1:C:52:GLU:CD	2.16	0.49
1:F:152:THR:HG23	1:F:154:ALA:H	1.76	0.49
1:E:152:THR:CG2	1:E:153:ARG:N	2.75	0.49
1:D:20:ILE:HD13	1:D:161:VAL:HG21	1.95	0.49
1:H:128:SER:HB2	1:H:134:ASP:O	2.11	0.49
3:E:4422:HOH:O	1:G:34:HIS:HD2	1.96	0.49
1:E:156:VAL:HA	1:F:159:GLN:HE22	1.77	0.49
1:A:86:SER:HB2	1:A:106:THR:HG23	1.94	0.49
1:D:4:MET:HB2	1:G:130:TYR:O	2.13	0.49
1:E:95:ASN:HD22	1:E:95:ASN:H	1.59	0.49
1:G:85:ASP:HA	1:G:114:LEU:CD2	2.43	0.49
1:D:16:LYS:HD3	1:D:78:ILE:HB	1.94	0.49
1:H:143:ILE:HD13	1:H:156:VAL:HG21	1.95	0.49
1:G:20:ILE:HG21	1:G:76:VAL:HG21	1.94	0.49
1:F:152:THR:HG23	1:F:154:ALA:N	2.28	0.49
1:G:112:VAL:HG23	1:G:113:ILE:N	2.28	0.49
1:E:123:LEU:O	1:E:126:VAL:HG12	2.13	0.49
1:C:91:VAL:HG12	1:C:102:ALA:O	2.13	0.49
1:A:46:GLU:HG2	3:A:4444:HOH:O	2.13	0.49
1:D:42:SER:HB3	1:D:61:ARG:NH2	2.28	0.49
1:A:95:ASN:ND2	1:A:98:GLN:N	2.56	0.48
1:E:166:SER:HB2	1:E:167:PRO:HD3	1.95	0.48
1:C:152:THR:HG22	1:C:155:SER:N	2.25	0.48
1:F:38:VAL:HG21	1:F:68:LEU:CD1	2.39	0.48
1:B:145:VAL:HG23	1:B:146:PHE:N	2.28	0.48
1:E:145:VAL:HG23	1:E:146:PHE:N	2.28	0.48
1:G:86:SER:HB3	1:G:108:PRO:HA	1.95	0.48
1:C:95:ASN:ND2	1:C:95:ASN:C	2.67	0.48
1:B:64:ASN:ND2	1:B:67:ARG:HH11	2.12	0.48
1:G:20:ILE:HD13	1:G:161:VAL:HG21	1.94	0.48
1:E:125:PRO:O	1:E:128:SER:HB2	2.13	0.48
1:H:126:VAL:HG13	1:H:127:MET:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:THR:HG23	3:D:4405:HOH:O	2.13	0.48
1:E:126:VAL:HG13	1:E:127:MET:N	2.28	0.48
1:G:112:VAL:O	1:G:115:GLU:HG2	2.13	0.48
1:G:159:GLN:NE2	3:H:4413:HOH:O	2.47	0.48
1:A:95:ASN:C	1:A:95:ASN:ND2	2.67	0.47
1:G:48:PRO:HB2	1:G:54:THR:HG22	1.95	0.47
1:F:116:LYS:NZ	1:F:129:ARG:NH2	2.57	0.47
1:A:27:ILE:CD1	1:A:165:LEU:HB3	2.45	0.47
1:D:20:ILE:HD11	1:D:78:ILE:HD11	1.94	0.47
1:A:172:VAL:C	1:A:174:SER:N	2.66	0.47
1:A:48:PRO:HB2	1:A:54:THR:HG22	1.96	0.47
1:E:152:THR:HG22	1:E:154:ALA:N	2.26	0.47
1:G:68:LEU:HB3	1:G:69:LEU:HD22	1.97	0.47
1:F:7:VAL:O	1:F:7:VAL:HG13	2.13	0.47
1:H:6:GLN:HG3	1:H:34:HIS:CE1	2.50	0.47
1:F:133:ILE:HG23	1:F:133:ILE:O	2.15	0.47
1:E:136:ILE:HD11	1:E:145:VAL:HG11	1.96	0.47
1:B:44:VAL:HG21	1:B:53:GLU:HG3	1.95	0.47
1:A:123:LEU:O	1:A:126:VAL:HG12	2.15	0.47
1:E:16:LYS:HD3	1:E:78:ILE:HB	1.97	0.47
1:G:157:TYR:O	1:G:161:VAL:HG23	2.14	0.47
1:B:172:VAL:C	1:B:174:SER:N	2.67	0.47
1:A:166:SER:HB2	1:A:167:PRO:HD3	1.97	0.47
1:B:93:ILE:HD13	1:B:165:LEU:HD22	1.95	0.47
1:H:83:ASP:HB2	1:H:88:PHE:CE2	2.40	0.47
1:G:82:ILE:CG2	1:G:83:ASP:N	2.78	0.47
1:A:9:CYS:O	1:A:37:SER:HA	2.15	0.47
1:C:133:ILE:HG12	3:C:4474:HOH:O	2.15	0.46
1:A:129:ARG:HB3	1:A:129:ARG:NH1	2.29	0.46
1:E:117:VAL:C	1:E:119:GLU:H	2.17	0.46
1:A:54:THR:HG21	1:A:81:GLY:HA3	1.98	0.46
1:F:76:VAL:HB	1:F:93:ILE:HG12	1.97	0.46
1:E:77:ALA:O	1:E:78:ILE:HD13	2.16	0.46
1:G:66:ARG:HA	1:G:75:TRP:NE1	2.31	0.46
1:F:109:LEU:CB	1:F:114:LEU:HD13	2.46	0.46
1:E:83:ASP:HB3	1:E:88:PHE:HE2	1.79	0.46
1:F:95:ASN:H	1:F:95:ASN:HD22	1.63	0.46
1:D:13:ASN:O	1:D:17:ILE:HG12	2.16	0.46
1:H:103:ARG:NH1	1:H:103:ARG:HG3	2.29	0.46
1:E:64:ASN:HD22	1:E:67:ARG:NH2	2.14	0.46
1:E:174:SER:HB2	3:E:4464:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:THR:HG22	1:H:153:ARG:N	2.31	0.45
1:A:47:GLN:HE21	1:A:123:LEU:H	1.64	0.45
1:H:87:THR:HB	1:H:109:LEU:HD11	1.98	0.45
1:H:20:ILE:HG21	1:H:76:VAL:HG11	1.98	0.45
1:C:110:PRO:HG2	1:C:113:ILE:HG13	1.99	0.45
1:A:118:ARG:HG2	1:A:118:ARG:HH11	1.81	0.45
1:C:95:ASN:HD22	1:C:95:ASN:C	2.19	0.45
1:G:38:VAL:HG21	1:G:68:LEU:CD2	2.44	0.45
1:C:133:ILE:CD1	1:C:139:LYS:HD2	2.34	0.45
1:E:20:ILE:HD11	1:E:78:ILE:HD11	1.98	0.45
1:E:93:ILE:O	1:E:99:ARG:HA	2.17	0.45
1:H:38:VAL:HG21	1:H:68:LEU:HD13	1.99	0.45
1:A:47:GLN:OE1	1:A:82:ILE:HD12	2.16	0.45
1:E:136:ILE:HD11	1:E:145:VAL:CG1	2.46	0.45
1:B:48:PRO:HG2	1:B:80:ALA:O	2.17	0.45
1:B:11:THR:HB	3:B:4448:HOH:O	2.16	0.45
1:B:147:THR:O	1:B:150:LYS:HG2	2.16	0.45
1:B:110:PRO:CG	1:B:113:ILE:HD13	2.44	0.45
1:F:117:VAL:HA	1:F:121:GLU:O	2.17	0.44
1:E:38:VAL:HG21	1:G:2:LEU:HD22	1.99	0.44
1:E:117:VAL:HA	1:E:121:GLU:O	2.17	0.44
1:F:145:VAL:CG2	1:F:146:PHE:N	2.80	0.44
1:H:71:GLU:HB2	3:H:4409:HOH:O	2.16	0.44
1:F:109:LEU:HB2	1:F:114:LEU:CD1	2.47	0.44
1:E:153:ARG:O	1:E:156:VAL:HG22	2.17	0.44
1:F:42:SER:O	1:F:60:ASN:HB2	2.18	0.44
1:E:145:VAL:CG2	1:E:146:PHE:N	2.80	0.44
1:H:20:ILE:HD12	1:H:76:VAL:HG21	2.00	0.44
1:G:127:MET:HE2	1:G:145:VAL:HG21	1.98	0.44
1:G:95:ASN:ND2	1:G:97:SER:H	2.15	0.44
1:B:47:GLN:HE21	1:B:123:LEU:H	1.64	0.44
1:H:13:ASN:O	1:H:17:ILE:HG12	2.18	0.44
1:F:36:ALA:HB2	3:F:4457:HOH:O	2.17	0.44
1:G:124:GLY:N	1:G:125:PRO:HD2	2.33	0.44
1:G:101:GLU:O	1:H:108:PRO:HG3	2.17	0.44
1:G:131:THR:HG22	1:G:132:GLY:N	2.33	0.44
1:B:98:GLN:HB2	1:B:168:PHE:CE1	2.52	0.44
1:A:82:ILE:N	1:A:82:ILE:HD13	2.30	0.44
1:G:27:ILE:HD12	1:G:165:LEU:HD23	2.00	0.44
1:C:2:LEU:N	1:C:2:LEU:HD23	2.33	0.44
1:H:99:ARG:NH2	3:H:4426:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:THR:CG2	1:H:153:ARG:N	2.80	0.43
1:A:21:LEU:HD13	1:A:35:ILE:HG23	2.00	0.43
1:F:119:GLU:HG3	3:F:4446:HOH:O	2.17	0.43
1:H:115:GLU:HG3	1:H:116:LYS:HD2	2.00	0.43
1:G:93:ILE:CD1	1:G:165:LEU:HD13	2.42	0.43
1:G:145:VAL:CG2	1:G:146:PHE:N	2.81	0.43
1:E:41:GLU:HG3	3:E:4438:HOH:O	2.18	0.43
1:D:95:ASN:HD22	1:D:98:GLN:H	1.56	0.43
1:B:67:ARG:HG3	1:B:67:ARG:HH21	1.83	0.43
1:C:133:ILE:HD13	1:C:133:ILE:C	2.38	0.43
1:G:103:ARG:HD3	1:H:103:ARG:NH1	2.34	0.43
1:G:172:VAL:HG22	1:G:172:VAL:O	2.19	0.43
1:G:21:LEU:HD13	1:G:35:ILE:HD11	2.01	0.43
1:C:161:VAL:O	1:C:165:LEU:HB2	2.18	0.43
1:C:153:ARG:NH2	2:C:4403:SO4:O1	2.50	0.43
1:A:71:GLU:HG2	3:A:4464:HOH:O	2.18	0.43
1:C:83:ASP:C	1:C:85:ASP:N	2.72	0.43
1:E:38:VAL:HG21	1:G:2:LEU:CD2	2.48	0.42
1:G:117:VAL:HG23	1:G:118:ARG:N	2.34	0.42
1:B:76:VAL:HG12	1:B:93:ILE:HG23	2.00	0.42
1:E:92:VAL:HG22	1:E:101:GLU:HG2	2.00	0.42
1:F:28:PHE:O	1:F:29:GLY:C	2.58	0.42
1:D:7:VAL:HG13	1:D:35:ILE:HG22	2.01	0.42
1:A:55:ARG:HB2	1:A:90:TRP:CD1	2.54	0.42
1:E:88:PHE:HB3	1:E:106:THR:HG22	2.01	0.42
1:C:133:ILE:HD13	1:C:134:ASP:O	2.19	0.42
1:H:7:VAL:CG1	1:H:35:ILE:HD12	2.49	0.42
1:E:5:HIS:HB3	1:E:73:ASP:OD1	2.20	0.42
1:F:129:ARG:HG2	1:F:129:ARG:O	2.19	0.42
1:E:64:ASN:ND2	1:E:67:ARG:NH2	2.67	0.42
1:C:8:VAL:HG23	1:C:72:ALA:CB	2.49	0.42
1:H:142:ALA:HA	1:H:145:VAL:HG13	2.01	0.42
1:C:133:ILE:O	1:C:133:ILE:HG23	2.20	0.42
1:F:45:PRO:HB2	3:F:4434:HOH:O	2.19	0.42
1:F:35:ILE:HG22	1:F:36:ALA:N	2.35	0.42
1:G:88:PHE:CE2	1:G:103:ARG:NH1	2.85	0.42
1:C:103:ARG:HD3	1:D:103:ARG:NH1	2.35	0.42
1:E:93:ILE:CD1	1:E:165:LEU:HD13	2.49	0.42
1:D:67:ARG:O	1:F:14:PRO:HB3	2.20	0.42
1:E:137:GLY:C	1:E:153:ARG:HH21	2.23	0.42
1:C:78:ILE:HD13	1:C:91:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:SER:HB3	1:D:61:ARG:CZ	2.50	0.42
1:H:94:GLU:CG	1:H:99:ARG:HD3	2.50	0.42
1:C:25:HIS:O	1:C:28:PHE:O	2.38	0.42
1:B:95:ASN:ND2	1:B:95:ASN:C	2.73	0.42
1:B:20:ILE:HD11	1:B:78:ILE:HD11	2.02	0.42
1:D:27:ILE:HG22	1:D:28:PHE:CD1	2.55	0.42
1:C:151:LEU:HD12	1:C:151:LEU:HA	1.79	0.42
1:C:4:MET:HB2	1:C:32:SER:O	2.20	0.42
1:B:129:ARG:HG3	3:B:4510:HOH:O	2.19	0.42
1:E:25:HIS:CD2	1:E:30:GLU:HG3	2.54	0.42
1:F:25:HIS:O	1:F:28:PHE:O	2.38	0.41
1:A:93:ILE:HD13	1:A:165:LEU:CD1	2.43	0.41
1:D:84:GLY:O	1:D:118:ARG:NH2	2.50	0.41
1:F:42:SER:HB3	1:F:61:ARG:CZ	2.51	0.41
1:G:140:GLU:O	1:G:141:GLY:O	2.39	0.41
1:A:55:ARG:HD2	3:A:4427:HOH:O	2.20	0.41
1:C:64:ASN:ND2	1:C:67:ARG:HH11	2.18	0.41
1:G:86:SER:HB2	1:G:107:LEU:O	2.20	0.41
1:D:172:VAL:HG22	1:D:172:VAL:O	2.21	0.41
1:B:54:THR:HG21	1:B:81:GLY:HA3	2.02	0.41
1:D:7:VAL:HG11	1:D:33:CYS:SG	2.61	0.41
1:H:34:HIS:CB	3:H:4408:HOH:O	2.68	0.41
1:H:166:SER:HB2	1:H:167:PRO:HD3	2.01	0.41
1:F:18:GLN:HB2	1:F:18:GLN:HE21	1.67	0.41
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.88	0.41
1:C:135:GLU:CG	1:C:138:ARG:HD3	2.39	0.41
1:F:20:ILE:HD12	1:F:76:VAL:CG2	2.49	0.41
1:F:159:GLN:NE2	3:F:4423:HOH:O	2.52	0.41
1:G:128:SER:C	1:G:130:TYR:H	2.24	0.41
1:C:13:ASN:O	1:C:17:ILE:HG12	2.20	0.41
1:F:108:PRO:HD3	3:F:4500:HOH:O	2.20	0.41
1:F:145:VAL:HG23	1:F:146:PHE:N	2.35	0.41
1:G:13:ASN:C	1:G:13:ASN:ND2	2.73	0.41
1:F:90:TRP:CE2	1:F:103:ARG:HG2	2.56	0.41
1:G:173:TYR:CE1	1:H:110:PRO:HG3	2.56	0.41
1:H:117:VAL:HA	1:H:121:GLU:O	2.20	0.41
1:E:47:GLN:HE21	1:E:47:GLN:CA	2.34	0.41
1:C:93:ILE:O	1:C:99:ARG:HA	2.21	0.41
1:B:173:TYR:O	1:B:174:SER:O	2.39	0.41
1:C:151:LEU:HD22	1:D:162:ILE:CG2	2.50	0.41
1:H:112:VAL:CG2	1:H:113:ILE:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ILE:CD1	1:E:91:VAL:HG23	2.51	0.40
1:B:143:ILE:HG12	3:B:4411:HOH:O	2.21	0.40
1:B:20:ILE:CG2	1:B:76:VAL:HG21	2.50	0.40
1:D:16:LYS:O	1:D:20:ILE:HG12	2.21	0.40
1:C:151:LEU:HD22	1:D:162:ILE:HG21	2.02	0.40
1:F:93:ILE:O	1:F:99:ARG:HA	2.22	0.40
1:G:119:GLU:HG3	1:G:119:GLU:O	2.21	0.40
1:A:159:GLN:HE22	1:B:156:VAL:HA	1.86	0.40
1:H:13:ASN:HD22	1:H:14:PRO:N	2.19	0.40
1:A:118:ARG:HA	1:A:118:ARG:CZ	2.52	0.40

All (4) 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:E:73:ASP:OD1	3:D:4457:HOH:O[1_455]	1.87	0.33
1:E:95:ASN:OD1	3:D:4409:HOH:O[1_455]	2.10	0.10
1:E:73:ASP:OD2	3:D:4444:HOH:O[1_455]	2.14	0.06
1:B:129:ARG:O	3:G:4452:HOH:O[1_656]	2.14	0.06

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	158/184 (86%)	151 (96%)	7 (4%)	0	100	100
1	B	170/184 (92%)	166 (98%)	4 (2%)	0	100	100
1	C	172/184 (94%)	164 (95%)	8 (5%)	0	100	100
1	D	170/184 (92%)	165 (97%)	5 (3%)	0	100	100
1	E	170/184 (92%)	159 (94%)	11 (6%)	0	100	100
1	F	170/184 (92%)	160 (94%)	8 (5%)	2 (1%)	16	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	164/184 (89%)	155 (94%)	8 (5%)	1 (1%)	30 36
1	H	168/184 (91%)	161 (96%)	6 (4%)	1 (1%)	30 36
All	All	1342/1472 (91%)	1281 (96%)	57 (4%)	4 (0%)	46 57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	134	ASP
1	F	29	GLY
1	G	141	GLY
1	F	130	TYR

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	124/144 (86%)	115 (93%)	9 (7%)	17 22
1	B	133/144 (92%)	126 (95%)	7 (5%)	28 37
1	C	134/144 (93%)	126 (94%)	8 (6%)	24 31
1	D	133/144 (92%)	128 (96%)	5 (4%)	40 54
1	E	133/144 (92%)	126 (95%)	7 (5%)	28 37
1	F	132/144 (92%)	124 (94%)	8 (6%)	23 30
1	G	130/144 (90%)	123 (95%)	7 (5%)	27 36
1	H	131/144 (91%)	119 (91%)	12 (9%)	11 13
All	All	1050/1152 (91%)	987 (94%)	63 (6%)	24 31

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	35	ILE
1	A	44	VAL

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Mol	Chain	Res	Type
1	A	46	GLU
1	A	82	ILE
1	A	83	ASP
1	A	95	ASN
1	A	116	LYS
1	A	165	LEU
1	B	3	ILE
1	B	44	VAL
1	B	54	THR
1	B	95	ASN
1	B	151	LEU
1	B	153	ARG
1	B	165	LEU
1	C	44	VAL
1	C	83	ASP
1	C	95	ASN
1	C	99	ARG
1	C	133	ILE
1	C	145	VAL
1	C	152	THR
1	C	165	LEU
1	D	6	GLN
1	D	95	ASN
1	D	116	LYS
1	D	152	THR
1	D	153	ARG
1	E	21	LEU
1	E	41	GLU
1	E	47	GLN
1	E	66	ARG
1	E	76	VAL
1	E	95	ASN
1	E	165	LEU
1	F	66	ARG
1	F	76	VAL
1	F	95	ASN
1	F	114	LEU
1	F	151	LEU
1	F	152	THR
1	F	153	ARG
1	F	165	LEU
1	G	2	LEU

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Mol	Chain	Res	Type
1	G	3	ILE
1	G	13	ASN
1	G	18	GLN
1	G	68	LEU
1	G	95	ASN
1	G	165	LEU
1	H	7	VAL
1	H	13	ASN
1	H	34	HIS
1	H	52	GLU
1	H	54	THR
1	H	85	ASP
1	H	95	ASN
1	H	99	ARG
1	H	114	LEU
1	H	116	LYS
1	H	145	VAL
1	H	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	18	GLN
1	A	22	GLN
1	A	64	ASN
1	A	95	ASN
1	A	98	GLN
1	A	159	GLN
1	B	18	GLN
1	B	22	GLN
1	B	47	GLN
1	B	64	ASN
1	B	95	ASN
1	C	64	ASN
1	C	95	ASN
1	C	159	GLN
1	D	22	GLN
1	D	60	ASN
1	D	95	ASN
1	D	159	GLN
1	D	170	ASN

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Mol	Chain	Res	Type
1	E	22	GLN
1	E	60	ASN
1	E	64	ASN
1	E	95	ASN
1	E	159	GLN
1	F	6	GLN
1	F	18	GLN
1	F	22	GLN
1	F	47	GLN
1	F	95	ASN
1	F	159	GLN
1	F	169	HIS
1	F	170	ASN
1	G	5	HIS
1	G	6	GLN
1	G	13	ASN
1	G	18	GLN
1	G	22	GLN
1	G	34	HIS
1	G	95	ASN
1	G	159	GLN
1	H	6	GLN
1	H	13	ASN
1	H	18	GLN
1	H	22	GLN
1	H	34	HIS
1	H	47	GLN
1	H	95	ASN
1	H	159	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 (i)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	4404	-	4,4,4	3.32	2 (50%)	6,6,6	0.92	0
2	SO4	B	4405	-	4,4,4	3.33	2 (50%)	6,6,6	0.94	0
2	SO4	B	4406	-	4,4,4	3.22	2 (50%)	6,6,6	0.98	0
2	SO4	B	4410	-	4,4,4	3.16	2 (50%)	6,6,6	0.98	0
2	SO4	C	4403	-	4,4,4	3.24	2 (50%)	6,6,6	0.96	0
2	SO4	C	4407	-	4,4,4	3.28	2 (50%)	6,6,6	0.93	0
2	SO4	D	4401	-	4,4,4	3.32	2 (50%)	6,6,6	1.00	0
2	SO4	D	4402	-	4,4,4	3.23	2 (50%)	6,6,6	0.97	0
2	SO4	E	4398	-	4,4,4	3.23	2 (50%)	6,6,6	1.01	0
2	SO4	E	4408	-	4,4,4	3.27	2 (50%)	6,6,6	0.97	0
2	SO4	F	4400	-	4,4,4	3.29	2 (50%)	6,6,6	0.96	0
2	SO4	F	4409	-	4,4,4	3.23	2 (50%)	6,6,6	0.98	0
2	SO4	G	4399	-	4,4,4	3.20	2 (50%)	6,6,6	1.00	0
2	SO4	H	4396	-	4,4,4	3.25	2 (50%)	6,6,6	0.97	0
2	SO4	H	4397	-	4,4,4	3.28	2 (50%)	6,6,6	1.00	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	A	4404	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4405	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4406	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4410	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4407	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	4401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4402	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4398	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4408	-	-	0/0/0/0	0/0/0/0
2	SO4	F	4400	-	-	0/0/0/0	0/0/0/0
2	SO4	F	4409	-	-	0/0/0/0	0/0/0/0
2	SO4	G	4399	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4396	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4397	-	-	0/0/0/0	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4401	SO4	O3-S	-4.72	1.30	1.47
2	H	4397	SO4	O3-S	-4.68	1.30	1.47
2	B	4406	SO4	O3-S	-4.64	1.30	1.47
2	B	4405	SO4	O3-S	-4.62	1.30	1.47
2	G	4399	SO4	O3-S	-4.60	1.30	1.47
2	F	4400	SO4	O3-S	-4.59	1.30	1.47
2	H	4396	SO4	O3-S	-4.57	1.30	1.47
2	E	4408	SO4	O3-S	-4.57	1.31	1.47
2	C	4403	SO4	O3-S	-4.55	1.31	1.47
2	A	4404	SO4	O3-S	-4.55	1.31	1.47
2	C	4407	SO4	O3-S	-4.51	1.31	1.47
2	F	4409	SO4	O3-S	-4.50	1.31	1.47
2	D	4402	SO4	O3-S	-4.47	1.31	1.47
2	E	4398	SO4	O3-S	-4.42	1.31	1.47
2	B	4410	SO4	O3-S	-4.00	1.33	1.47
2	B	4406	SO4	O1-S	4.36	1.62	1.47
2	G	4399	SO4	O1-S	4.37	1.62	1.47
2	C	4403	SO4	O1-S	4.46	1.62	1.47
2	H	4397	SO4	O1-S	4.47	1.62	1.47
2	H	4396	SO4	O1-S	4.54	1.62	1.47
2	D	4401	SO4	O1-S	4.54	1.62	1.47
2	F	4409	SO4	O1-S	4.56	1.62	1.47
2	D	4402	SO4	O1-S	4.56	1.62	1.47
2	E	4408	SO4	O1-S	4.59	1.62	1.47
2	F	4400	SO4	O1-S	4.60	1.62	1.47
2	E	4398	SO4	O1-S	4.66	1.63	1.47
2	C	4407	SO4	O1-S	4.69	1.63	1.47
2	B	4410	SO4	O1-S	4.71	1.63	1.47
2	B	4405	SO4	O1-S	4.71	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4404	SO4	O1-S	4.74	1.63	1.47

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	C	4403	SO4	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	162/184 (88%)	0.78	11 (6%) 20 28	17, 30, 63, 82	0
1	B	172/184 (93%)	0.26	4 (2%) 64 72	12, 25, 45, 59	0
1	C	174/184 (94%)	0.65	13 (7%) 17 24	12, 28, 45, 66	0
1	D	172/184 (93%)	0.23	5 (2%) 55 64	14, 25, 44, 54	0
1	E	172/184 (93%)	0.75	12 (6%) 19 27	18, 28, 55, 65	0
1	F	172/184 (93%)	0.07	3 (1%) 73 79	18, 28, 51, 60	0
1	G	168/184 (91%)	0.83	19 (11%) 7 10	16, 29, 64, 73	0
1	H	170/184 (92%)	0.17	4 (2%) 62 71	16, 29, 58, 69	0
All	All	1362/1472 (92%)	0.47	71 (5%) 31 39	12, 28, 55, 82	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ILE	5.5
1	C	29	GLY	4.4
1	A	129	ARG	3.9
1	G	174	SER	3.9
1	G	114	LEU	3.7
1	E	49	PHE	3.6
1	G	2	LEU	3.5
1	E	67	ARG	3.4
1	G	38	VAL	3.2
1	A	4	MET	3.2
1	C	2	LEU	3.2
1	H	134	ASP	3.1
1	E	70	PRO	3.1
1	C	171	ALA	3.0
1	E	3	ILE	3.0
1	G	132	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	133	ILE	2.9
1	D	117	VAL	2.9
1	A	36	ALA	2.9
1	G	116	LYS	2.8
1	E	174	SER	2.8
1	C	7	VAL	2.8
1	A	8	VAL	2.7
1	G	117	VAL	2.7
1	E	133	ILE	2.7
1	G	129	ARG	2.7
1	A	128	SER	2.7
1	A	74	PHE	2.6
1	A	6	GLN	2.6
1	G	118	ARG	2.5
1	E	38	VAL	2.5
1	C	96	ALA	2.5
1	B	110	PRO	2.5
1	C	74	PHE	2.5
1	D	112	VAL	2.5
1	E	138	ARG	2.4
1	E	134	ASP	2.4
1	D	33	CYS	2.4
1	C	5	HIS	2.4
1	E	4	MET	2.4
1	H	128	SER	2.4
1	G	57	GLY	2.4
1	C	168	PHE	2.3
1	A	69	LEU	2.3
1	E	68	LEU	2.3
1	G	10	ALA	2.3
1	A	28	PHE	2.3
1	F	133	ILE	2.3
1	D	115	GLU	2.3
1	B	32	SER	2.3
1	C	43	GLY	2.2
1	G	67	ARG	2.2
1	G	68	LEU	2.2
1	G	121	GLU	2.2
1	C	34	HIS	2.2
1	C	67	ARG	2.2
1	G	43	GLY	2.2
1	C	33	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	131	THR	2.2
1	D	136	ILE	2.2
1	B	33	CYS	2.2
1	H	130	TYR	2.1
1	F	131	THR	2.1
1	E	33	CYS	2.1
1	G	126	VAL	2.1
1	H	131	THR	2.1
1	B	132	GLY	2.1
1	A	34	HIS	2.1
1	G	11	THR	2.0
1	F	112	VAL	2.0
1	A	72	ALA	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	E	4408	5/5	0.70	0.23	2.90	97,98,98,99	0
2	SO4	H	4397	5/5	0.94	0.14	1.82	52,52,53,53	0
2	SO4	G	4399	5/5	0.93	0.26	1.69	46,46,48,48	0
2	SO4	B	4406	5/5	0.95	0.16	1.33	37,37,39,40	0
2	SO4	F	4409	5/5	0.85	0.16	1.24	80,81,81,81	0
2	SO4	F	4400	5/5	0.94	0.14	1.13	59,60,61,61	0
2	SO4	D	4402	5/5	0.91	0.15	0.42	47,48,48,49	0
2	SO4	H	4396	5/5	0.91	0.14	0.17	73,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	4410	5/5	0.96	0.13	-0.02	18,19,20,21	0
2	SO4	C	4407	5/5	0.90	0.15	-0.26	48,48,51,51	0
2	SO4	D	4401	5/5	0.96	0.13	-0.36	28,29,32,32	0
2	SO4	B	4405	5/5	0.95	0.13	-0.43	43,44,46,46	0
2	SO4	C	4403	5/5	0.95	0.13	-0.67	35,36,36,37	0
2	SO4	A	4404	5/5	0.94	0.11	-1.99	51,52,53,53	0
2	SO4	E	4398	5/5	0.95	0.12	-2.53	35,36,39,40	0

6.5 Other polymers

There are no such residues in this entry.