Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:32 AM GMT

PDB ID	:	3EZZ
Title	:	Crystal Structure of human MKP-2
Authors	:	Jeong, D.G.; Jung, S.K.; Ryu, S.E.; Kim, S.J.
Deposited on	:	2008-10-24
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
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:

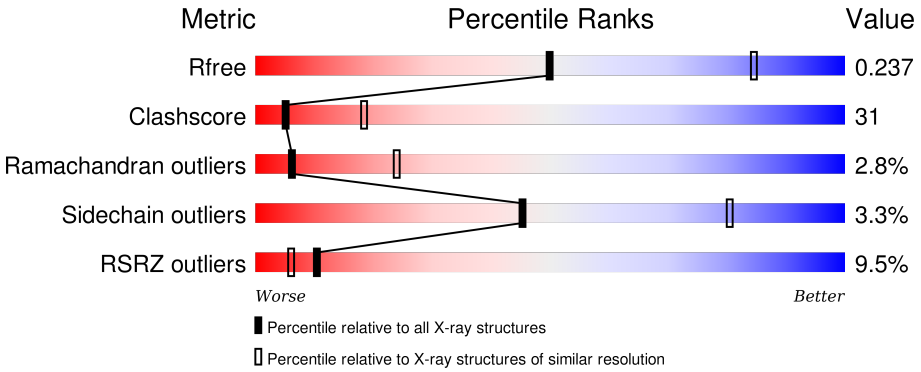
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 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	144	8% 50% 47% ·
1	B	144	4% 47% 51% ·
1	C	144	11% 51% 44% 5%
1	D	144	17% 50% 47% ·
1	E	144	7% 46% 51% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	144	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6921 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.

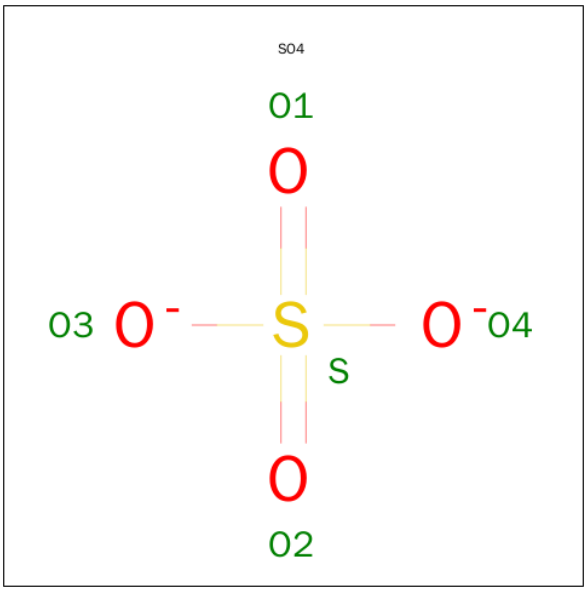
- Molecule 1 is a protein called Dual specificity protein phosphatase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			
1	B	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			
1	C	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			
1	D	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			
1	E	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			
1	F	144	Total	C	N	O	S	0	0	0
			1146	731	198	207	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	MET	-	INITIATING METHIONINE	UNP Q13115
A	280	SER	CYS	ENGINEERED	UNP Q13115
B	193	MET	-	INITIATING METHIONINE	UNP Q13115
B	280	SER	CYS	ENGINEERED	UNP Q13115
C	193	MET	-	INITIATING METHIONINE	UNP Q13115
C	280	SER	CYS	ENGINEERED	UNP Q13115
D	193	MET	-	INITIATING METHIONINE	UNP Q13115
D	280	SER	CYS	ENGINEERED	UNP Q13115
E	193	MET	-	INITIATING METHIONINE	UNP Q13115
E	280	SER	CYS	ENGINEERED	UNP Q13115
F	193	MET	-	INITIATING METHIONINE	UNP Q13115
F	280	SER	CYS	ENGINEERED	UNP Q13115

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



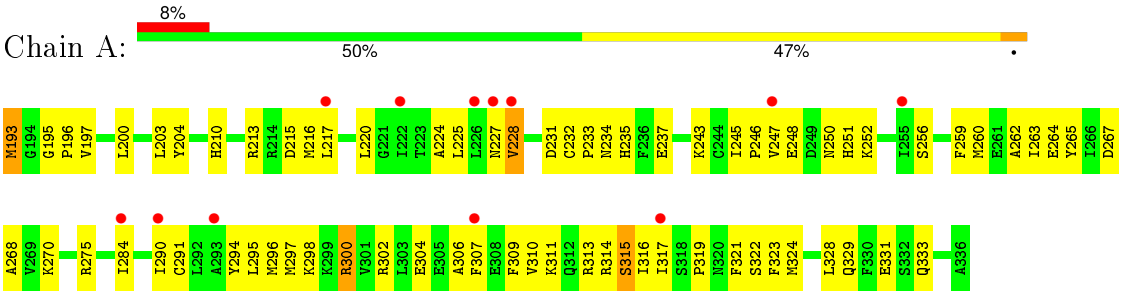
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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.

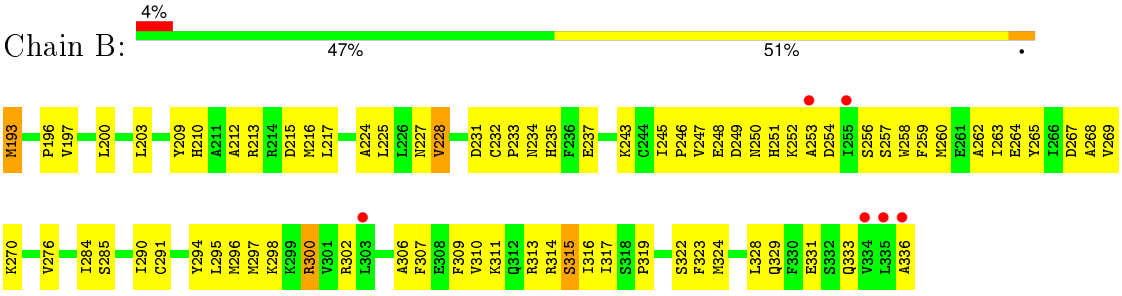
- Molecule 1: Dual specificity protein phosphatase 4

Chain A:



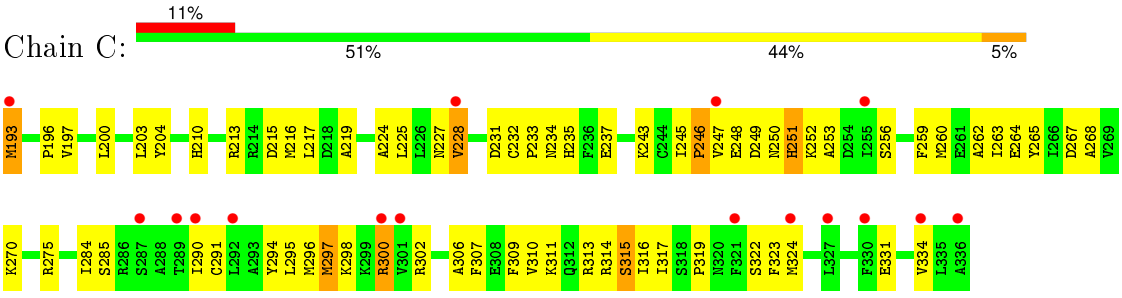
- Molecule 1: Dual specificity protein phosphatase 4

Chain B:



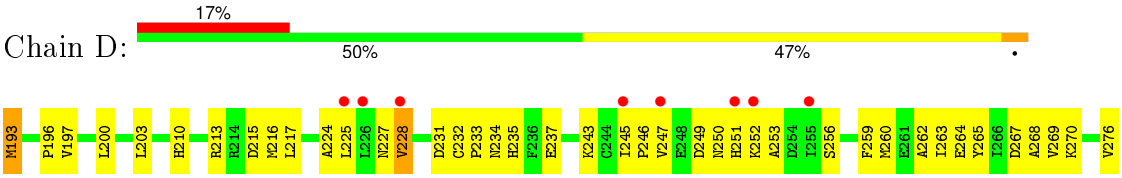
- Molecule 1: Dual specificity protein phosphatase 4

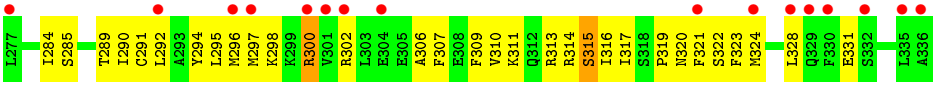
Chain C:



- Molecule 1: Dual specificity protein phosphatase 4

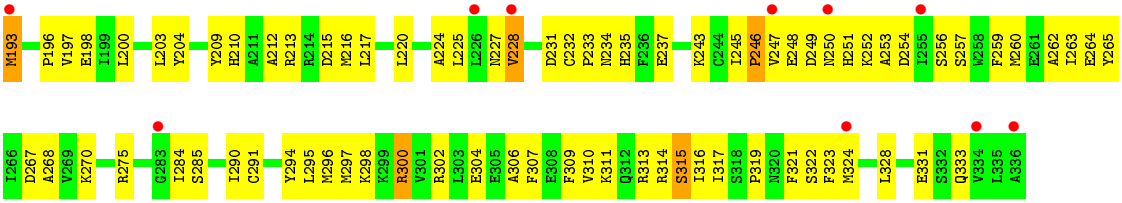
Chain D:





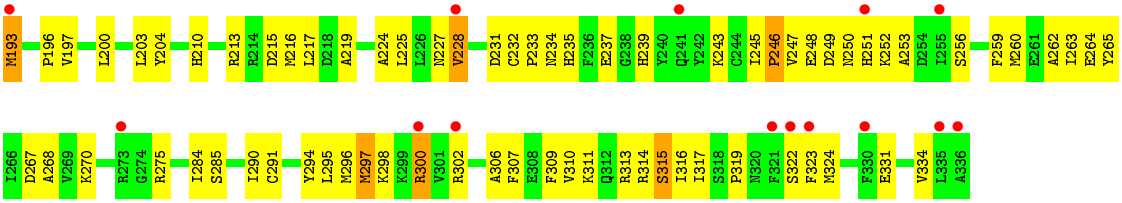
• Molecule 1: Dual specificity protein phosphatase 4

Chain E:



• Molecule 1: Dual specificity protein phosphatase 4

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	141.56Å 141.56Å 158.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 79.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.90) 99.9 (79.27-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.91Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	0.219 , 0.242 0.218 , 0.237	Depositor DCC
R_{free} test set	1688 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	74.8	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.8	EDS
Estimated twinning fraction	0.378 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 34516 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6921	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0/1171	0.65	0/1577
1	B	0.46	0/1171	0.66	0/1577
1	C	0.53	1/1171 (0.1%)	0.67	1/1577 (0.1%)
1	D	0.49	0/1171	0.67	0/1577
1	E	0.45	0/1171	0.66	0/1577
1	F	0.49	0/1171	0.66	0/1577
All	All	0.48	1/7026 (0.0%)	0.66	1/9462 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	HIS	C-O	-5.71	1.12	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	251	HIS	CA-C-N	-5.82	104.39	117.20

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	1146	0	1136	81	0
1	B	1146	0	1136	78	0
1	C	1146	0	1136	68	0
1	D	1146	0	1136	65	0
1	E	1146	0	1136	87	0
1	F	1146	0	1136	71	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
All	All	6921	0	6816	422	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 31.

All (422) 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:304:GLU:HA	1:E:321:PHE:CE1	1.69	1.26
1:B:333:GLN:HB3	1:E:333:GLN:OE1	1.47	1.12
1:A:304:GLU:HA	1:E:321:PHE:HE1	0.96	1.06
1:A:298:LYS:HE2	1:A:298:LYS:HA	1.43	1.00
1:E:298:LYS:HA	1:E:298:LYS:HE2	1.42	1.00
1:B:298:LYS:HE2	1:B:298:LYS:HA	1.44	1.00
1:F:298:LYS:HE2	1:F:298:LYS:HA	1.45	0.99
1:B:336:ALA:HB2	1:E:260:MET:SD	2.03	0.99
1:B:336:ALA:CB	1:E:260:MET:SD	2.51	0.97
1:C:298:LYS:HE2	1:C:298:LYS:HA	1.46	0.97
1:D:298:LYS:HA	1:D:298:LYS:HE2	1.46	0.95
1:E:310:VAL:HG12	1:E:317:ILE:HD11	1.54	0.89
1:A:227:ASN:HD21	1:A:232:CYS:HB3	1.39	0.87
1:A:310:VAL:HG12	1:A:317:ILE:HD11	1.57	0.85
1:E:316:ILE:HD12	1:E:316:ILE:H	1.39	0.85
1:C:316:ILE:HD12	1:C:316:ILE:H	1.40	0.85
1:D:310:VAL:HG12	1:D:317:ILE:HD11	1.59	0.85
1:D:227:ASN:HD21	1:D:232:CYS:HB3	1.41	0.85
1:B:310:VAL:HG12	1:B:317:ILE:HD11	1.57	0.84
1:B:227:ASN:HD21	1:B:232:CYS:HB3	1.43	0.83
1:C:227:ASN:HD21	1:C:232:CYS:HB3	1.44	0.83
1:B:316:ILE:H	1:B:316:ILE:HD12	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASN:HD21	1:E:232:CYS:HB3	1.42	0.83
1:A:321:PHE:CE1	1:E:304:GLU:HA	2.14	0.82
1:F:316:ILE:HD12	1:F:316:ILE:H	1.42	0.82
1:D:316:ILE:H	1:D:316:ILE:HD12	1.43	0.82
1:A:304:GLU:CA	1:E:321:PHE:HE1	1.88	0.81
1:C:310:VAL:HG12	1:C:317:ILE:HD11	1.60	0.81
1:A:316:ILE:H	1:A:316:ILE:HD12	1.46	0.81
1:B:333:GLN:CB	1:E:333:GLN:OE1	2.28	0.81
1:B:336:ALA:HB1	1:E:260:MET:SD	2.22	0.80
1:A:304:GLU:CA	1:E:321:PHE:CE1	2.61	0.80
1:F:310:VAL:HG12	1:F:317:ILE:HD11	1.62	0.80
1:E:294:TYR:CZ	1:E:298:LYS:HG3	2.16	0.80
1:F:227:ASN:HD21	1:F:232:CYS:HB3	1.47	0.78
1:B:200:LEU:HB2	1:B:203:LEU:HB3	1.66	0.77
1:D:200:LEU:HB2	1:D:203:LEU:HB3	1.66	0.77
1:D:294:TYR:CZ	1:D:298:LYS:HG3	2.20	0.77
1:A:321:PHE:HE1	1:E:304:GLU:HA	1.50	0.76
1:B:294:TYR:CZ	1:B:298:LYS:HG3	2.20	0.76
1:C:294:TYR:CZ	1:C:298:LYS:HG3	2.21	0.76
1:B:314:ARG:O	1:B:317:ILE:HG13	1.87	0.75
1:D:314:ARG:O	1:D:317:ILE:HG13	1.86	0.75
1:F:200:LEU:HB2	1:F:203:LEU:HB3	1.67	0.75
1:E:200:LEU:HB2	1:E:203:LEU:HB3	1.69	0.74
1:D:251:HIS:HA	1:D:322:SER:CB	2.17	0.74
1:F:314:ARG:O	1:F:317:ILE:HG13	1.88	0.73
1:C:200:LEU:HB2	1:C:203:LEU:HB3	1.67	0.73
1:A:200:LEU:HB2	1:A:203:LEU:HB3	1.69	0.73
1:F:251:HIS:HA	1:F:322:SER:CB	2.19	0.73
1:E:314:ARG:O	1:E:317:ILE:HG13	1.89	0.73
1:A:294:TYR:CZ	1:A:298:LYS:HG3	2.23	0.73
1:F:294:TYR:CZ	1:F:298:LYS:HG3	2.23	0.73
1:C:314:ARG:O	1:C:317:ILE:HG13	1.88	0.72
1:A:314:ARG:O	1:A:317:ILE:HG13	1.91	0.71
1:A:251:HIS:HA	1:A:322:SER:CB	2.20	0.71
1:B:251:HIS:HA	1:B:322:SER:CB	2.21	0.71
1:E:251:HIS:HA	1:E:322:SER:CB	2.21	0.70
1:A:296:MET:O	1:A:300:ARG:HA	1.92	0.70
1:D:296:MET:O	1:D:300:ARG:HA	1.92	0.70
1:C:316:ILE:HD12	1:C:316:ILE:N	2.07	0.70
1:F:296:MET:O	1:F:300:ARG:HA	1.91	0.69
1:C:296:MET:O	1:C:300:ARG:HA	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:ILE:HD12	1:E:316:ILE:N	2.08	0.69
1:B:197:VAL:HG11	1:B:313:ARG:HB3	1.75	0.69
1:B:296:MET:O	1:B:300:ARG:HA	1.94	0.68
1:E:296:MET:O	1:E:300:ARG:HA	1.93	0.68
1:F:197:VAL:HG11	1:F:313:ARG:HB3	1.76	0.67
1:E:197:VAL:HG11	1:E:313:ARG:HB3	1.75	0.67
1:F:316:ILE:N	1:F:316:ILE:HD12	2.08	0.67
1:D:251:HIS:HA	1:D:322:SER:HB2	1.75	0.67
1:C:319:PRO:HB2	1:C:324:MET:HE1	1.77	0.66
1:C:251:HIS:HA	1:C:322:SER:CB	2.26	0.66
1:B:316:ILE:N	1:B:316:ILE:HD12	2.10	0.66
1:D:316:ILE:HD12	1:D:316:ILE:N	2.09	0.65
1:C:197:VAL:HG11	1:C:313:ARG:HB3	1.78	0.65
1:F:228:VAL:O	1:F:228:VAL:HG12	1.97	0.64
1:D:197:VAL:HG11	1:D:313:ARG:HB3	1.78	0.64
1:F:251:HIS:HA	1:F:322:SER:HB2	1.79	0.64
1:A:316:ILE:N	1:A:316:ILE:HD12	2.12	0.64
1:E:228:VAL:HG12	1:E:228:VAL:O	1.98	0.64
1:A:197:VAL:HG11	1:A:313:ARG:HB3	1.79	0.64
1:A:319:PRO:HB2	1:A:324:MET:HE1	1.80	0.63
1:A:259:PHE:O	1:A:263:ILE:HG13	1.99	0.62
1:F:319:PRO:HB2	1:F:324:MET:HE1	1.81	0.62
1:E:319:PRO:HB2	1:E:324:MET:HE1	1.81	0.62
1:E:251:HIS:HA	1:E:322:SER:HB2	1.80	0.62
1:E:316:ILE:H	1:E:316:ILE:CD1	2.12	0.61
1:A:228:VAL:O	1:A:228:VAL:HG12	2.00	0.61
1:D:259:PHE:O	1:D:263:ILE:HG13	2.01	0.61
1:D:319:PRO:HB2	1:D:324:MET:HE1	1.82	0.60
1:C:291:CYS:O	1:C:295:LEU:HG	2.02	0.60
1:B:251:HIS:HA	1:B:322:SER:HB2	1.82	0.60
1:D:256:SER:HA	1:D:259:PHE:CE2	2.36	0.60
1:E:196:PRO:HG3	1:E:210:HIS:ND1	2.17	0.60
1:C:256:SER:HA	1:C:259:PHE:CE2	2.37	0.60
1:B:256:SER:HA	1:B:259:PHE:CE2	2.37	0.60
1:B:228:VAL:O	1:B:228:VAL:HG12	2.01	0.59
1:A:251:HIS:HA	1:A:322:SER:HB2	1.82	0.59
1:F:259:PHE:O	1:F:263:ILE:HG13	2.02	0.59
1:C:228:VAL:HG12	1:C:228:VAL:O	2.02	0.59
1:D:267:ASP:O	1:D:270:LYS:HB3	2.03	0.59
1:E:291:CYS:O	1:E:295:LEU:HG	2.02	0.59
1:F:291:CYS:O	1:F:295:LEU:HG	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:ARG:HD3	1:F:313:ARG:N	2.17	0.58
1:E:196:PRO:HG3	1:E:210:HIS:HD1	1.67	0.58
1:E:224:ALA:C	1:E:225:LEU:HD12	2.23	0.58
1:B:319:PRO:HB2	1:B:324:MET:HE1	1.84	0.58
1:C:313:ARG:HD3	1:C:313:ARG:N	2.18	0.58
1:F:316:ILE:H	1:F:316:ILE:CD1	2.15	0.58
1:C:316:ILE:CD1	1:C:316:ILE:H	2.13	0.58
1:C:302:ARG:HD3	1:C:331:GLU:OE1	2.03	0.58
1:B:291:CYS:O	1:B:295:LEU:HG	2.03	0.57
1:E:256:SER:HA	1:E:259:PHE:CE2	2.40	0.57
1:E:313:ARG:HD3	1:E:313:ARG:N	2.20	0.57
1:B:196:PRO:HG3	1:B:210:HIS:ND1	2.20	0.57
1:F:256:SER:HA	1:F:259:PHE:CE2	2.39	0.57
1:B:329:GLN:CD	1:E:254:ASP:OD1	2.43	0.57
1:A:329:GLN:NE2	1:B:258:TRP:CZ3	2.72	0.57
1:D:228:VAL:HG12	1:D:228:VAL:O	2.05	0.57
1:A:321:PHE:HE1	1:E:304:GLU:CA	2.15	0.57
1:A:250:ASN:HB3	1:A:252:LYS:H	1.69	0.57
1:A:313:ARG:N	1:A:313:ARG:HD3	2.20	0.57
1:A:256:SER:HA	1:A:259:PHE:CE2	2.40	0.57
1:E:260:MET:O	1:E:264:GLU:HG3	2.05	0.56
1:D:196:PRO:HG3	1:D:210:HIS:HD1	1.70	0.56
1:D:196:PRO:HG3	1:D:210:HIS:ND1	2.19	0.56
1:E:259:PHE:O	1:E:263:ILE:HG13	2.05	0.56
1:B:196:PRO:HG3	1:B:210:HIS:HD1	1.71	0.56
1:D:302:ARG:HD3	1:D:331:GLU:OE1	2.06	0.56
1:A:298:LYS:CA	1:A:298:LYS:HE2	2.28	0.56
1:D:316:ILE:CD1	1:D:316:ILE:H	2.15	0.56
1:D:234:ASN:O	1:D:237:GLU:HG2	2.06	0.56
1:D:306:ALA:O	1:D:310:VAL:HG23	2.06	0.56
1:B:316:ILE:CD1	1:B:316:ILE:H	2.16	0.56
1:B:313:ARG:N	1:B:313:ARG:HD3	2.21	0.55
1:C:250:ASN:HB3	1:C:252:LYS:H	1.71	0.55
1:D:313:ARG:HD3	1:D:313:ARG:N	2.20	0.55
1:F:302:ARG:HD3	1:F:331:GLU:OE1	2.05	0.55
1:F:265:TYR:O	1:F:268:ALA:HB3	2.06	0.55
1:D:291:CYS:O	1:D:295:LEU:HG	2.06	0.55
1:D:311:LYS:HA	1:D:317:ILE:HD12	1.88	0.55
1:A:321:PHE:CE1	1:E:304:GLU:CA	2.89	0.55
1:A:304:GLU:HA	1:E:321:PHE:CD1	2.38	0.55
1:A:309:PHE:CE1	1:A:313:ARG:NH2	2.74	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:O	1:B:237:GLU:HG2	2.06	0.55
1:B:328:LEU:HD11	1:D:321:PHE:HB3	1.89	0.55
1:E:302:ARG:HD3	1:E:331:GLU:OE1	2.06	0.55
1:B:250:ASN:HB3	1:B:252:LYS:H	1.72	0.55
1:D:309:PHE:CE1	1:D:313:ARG:NH2	2.75	0.55
1:C:234:ASN:O	1:C:237:GLU:HG2	2.06	0.55
1:F:251:HIS:NE2	1:F:252:LYS:HE3	2.22	0.55
1:A:196:PRO:HG3	1:A:210:HIS:ND1	2.22	0.55
1:A:291:CYS:O	1:A:295:LEU:HG	2.08	0.54
1:B:267:ASP:O	1:B:270:LYS:HB3	2.07	0.54
1:A:234:ASN:O	1:A:237:GLU:HG2	2.07	0.54
1:F:234:ASN:O	1:F:237:GLU:HG2	2.06	0.54
1:A:260:MET:O	1:A:264:GLU:HG3	2.08	0.54
1:C:311:LYS:HA	1:C:317:ILE:HD12	1.89	0.54
1:E:250:ASN:HB3	1:E:252:LYS:H	1.71	0.54
1:A:196:PRO:HG3	1:A:210:HIS:HD1	1.73	0.54
1:F:260:MET:O	1:F:264:GLU:HG3	2.07	0.54
1:E:306:ALA:O	1:E:310:VAL:HG23	2.07	0.54
1:E:234:ASN:O	1:E:237:GLU:HG2	2.06	0.54
1:A:302:ARG:HD3	1:A:331:GLU:OE1	2.07	0.54
1:B:298:LYS:CA	1:B:298:LYS:HE2	2.29	0.54
1:A:251:HIS:NE2	1:A:252:LYS:HE3	2.22	0.54
1:B:265:TYR:O	1:B:268:ALA:HB3	2.08	0.54
1:E:265:TYR:O	1:E:268:ALA:HB3	2.08	0.54
1:C:260:MET:O	1:C:264:GLU:HG3	2.08	0.54
1:C:306:ALA:O	1:C:310:VAL:HG23	2.08	0.53
1:D:224:ALA:C	1:D:225:LEU:HD12	2.28	0.53
1:F:250:ASN:HB3	1:F:252:LYS:H	1.72	0.53
1:C:309:PHE:CE1	1:C:313:ARG:NH2	2.76	0.53
1:F:245:ILE:O	1:F:247:VAL:HG23	2.08	0.53
1:A:265:TYR:O	1:A:268:ALA:HB3	2.08	0.53
1:A:267:ASP:O	1:A:270:LYS:HB3	2.07	0.53
1:D:265:TYR:O	1:D:268:ALA:HB3	2.07	0.53
1:A:224:ALA:C	1:A:225:LEU:HD12	2.29	0.53
1:B:245:ILE:O	1:B:247:VAL:HG23	2.07	0.53
1:C:298:LYS:CA	1:C:298:LYS:HE2	2.30	0.53
1:B:306:ALA:O	1:B:310:VAL:HG23	2.08	0.53
1:B:259:PHE:O	1:B:263:ILE:HG13	2.09	0.53
1:A:333:GLN:NE2	1:B:258:TRP:CZ2	2.76	0.53
1:E:245:ILE:CD1	1:E:262:ALA:HB2	2.38	0.53
1:F:311:LYS:HA	1:F:317:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ASN:HB3	1:D:252:LYS:H	1.73	0.53
1:D:243:LYS:HB2	1:D:265:TYR:CE1	2.42	0.53
1:E:243:LYS:HB2	1:E:265:TYR:CE1	2.43	0.53
1:D:251:HIS:NE2	1:D:252:LYS:HE3	2.24	0.53
1:C:259:PHE:O	1:C:263:ILE:HG13	2.09	0.53
1:B:224:ALA:C	1:B:225:LEU:HD12	2.29	0.53
1:A:311:LYS:HA	1:A:317:ILE:HD12	1.91	0.53
1:C:243:LYS:HB2	1:C:265:TYR:CE1	2.44	0.53
1:A:316:ILE:H	1:A:316:ILE:CD1	2.18	0.53
1:A:243:LYS:HB2	1:A:265:TYR:CE1	2.43	0.53
1:C:265:TYR:O	1:C:268:ALA:HB3	2.09	0.53
1:C:196:PRO:HG3	1:C:210:HIS:ND1	2.24	0.52
1:F:196:PRO:HG3	1:F:210:HIS:ND1	2.25	0.52
1:F:267:ASP:O	1:F:270:LYS:HB3	2.09	0.52
1:B:260:MET:O	1:B:264:GLU:HG3	2.10	0.52
1:B:243:LYS:HB2	1:B:265:TYR:CE1	2.44	0.52
1:B:302:ARG:HD3	1:B:331:GLU:OE1	2.10	0.52
1:D:245:ILE:CD1	1:D:262:ALA:HB2	2.40	0.52
1:E:233:PRO:HB2	1:E:235:HIS:CE1	2.45	0.52
1:B:251:HIS:NE2	1:B:252:LYS:HE3	2.25	0.52
1:C:224:ALA:C	1:C:225:LEU:HD12	2.30	0.52
1:E:267:ASP:O	1:E:270:LYS:HB3	2.09	0.51
1:E:310:VAL:CG1	1:E:317:ILE:HD11	2.35	0.51
1:B:197:VAL:CG1	1:B:313:ARG:HB3	2.41	0.51
1:E:245:ILE:O	1:E:247:VAL:HG23	2.10	0.51
1:B:245:ILE:CD1	1:B:262:ALA:HB2	2.41	0.51
1:C:267:ASP:O	1:C:270:LYS:HB3	2.11	0.51
1:D:298:LYS:CA	1:D:298:LYS:HE2	2.31	0.51
1:A:227:ASN:ND2	1:A:232:CYS:HB3	2.19	0.50
1:E:251:HIS:NE2	1:E:252:LYS:HE3	2.26	0.50
1:B:215:ASP:OD1	1:B:216:MET:N	2.44	0.50
1:A:306:ALA:O	1:A:310:VAL:HG23	2.11	0.50
1:D:260:MET:O	1:D:264:GLU:HG3	2.11	0.50
1:A:245:ILE:O	1:A:247:VAL:HG23	2.12	0.50
1:F:224:ALA:C	1:F:225:LEU:HD12	2.31	0.50
1:D:284:ILE:HG23	1:D:316:ILE:O	2.12	0.50
1:A:197:VAL:CG1	1:A:313:ARG:HB3	2.41	0.50
1:C:284:ILE:HG23	1:C:316:ILE:O	2.12	0.49
1:F:197:VAL:CG1	1:F:313:ARG:HB3	2.41	0.49
1:B:209:TYR:HB2	1:C:219:ALA:HB2	1.95	0.49
1:E:197:VAL:CG1	1:E:313:ARG:HB3	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:ILE:HG22	1:F:247:VAL:HG23	1.94	0.49
1:A:310:VAL:CG1	1:A:317:ILE:HD11	2.37	0.49
1:B:227:ASN:ND2	1:B:232:CYS:HB3	2.22	0.49
1:F:306:ALA:O	1:F:310:VAL:HG23	2.12	0.49
1:C:251:HIS:HA	1:C:322:SER:HB2	1.94	0.49
1:C:196:PRO:HG3	1:C:210:HIS:HD1	1.78	0.49
1:E:311:LYS:HA	1:E:317:ILE:HD12	1.94	0.49
1:F:243:LYS:HB2	1:F:265:TYR:CE1	2.47	0.49
1:D:245:ILE:HG22	1:D:247:VAL:HG23	1.95	0.49
1:B:311:LYS:HA	1:B:317:ILE:HD12	1.94	0.49
1:F:309:PHE:CE1	1:F:313:ARG:NH2	2.81	0.49
1:C:228:VAL:CG1	1:C:290:ILE:HD12	2.43	0.49
1:C:256:SER:HA	1:C:259:PHE:CD2	2.47	0.49
1:C:245:ILE:O	1:C:247:VAL:HG23	2.12	0.49
1:A:228:VAL:HG11	1:A:290:ILE:HD12	1.95	0.48
1:C:197:VAL:CG1	1:C:313:ARG:HB3	2.43	0.48
1:D:197:VAL:CG1	1:D:313:ARG:HB3	2.42	0.48
1:E:298:LYS:HE2	1:E:298:LYS:CA	2.28	0.48
1:A:193:MET:HA	1:A:210:HIS:NE2	2.29	0.48
1:C:213:ARG:O	1:C:217:LEU:HG	2.13	0.48
1:E:215:ASP:OD1	1:E:216:MET:N	2.46	0.48
1:D:233:PRO:HB2	1:D:235:HIS:CE1	2.49	0.48
1:B:233:PRO:HB2	1:B:235:HIS:CE1	2.49	0.48
1:E:193:MET:HA	1:E:210:HIS:NE2	2.29	0.48
1:A:333:GLN:NE2	1:B:258:TRP:HZ2	2.11	0.48
1:D:215:ASP:OD1	1:D:216:MET:N	2.47	0.48
1:B:213:ARG:O	1:B:217:LEU:HG	2.14	0.48
1:B:256:SER:HA	1:B:259:PHE:CD2	2.49	0.47
1:B:193:MET:HA	1:B:210:HIS:NE2	2.29	0.47
1:B:245:ILE:HG22	1:B:247:VAL:HG23	1.96	0.47
1:B:310:VAL:CG1	1:B:317:ILE:HD11	2.38	0.47
1:A:321:PHE:HE1	1:E:304:GLU:CB	2.26	0.47
1:D:228:VAL:HG11	1:D:290:ILE:HD12	1.96	0.47
1:E:245:ILE:HG22	1:E:247:VAL:HG23	1.96	0.47
1:C:233:PRO:HB2	1:C:235:HIS:CE1	2.49	0.47
1:C:297:MET:HE3	1:C:334:VAL:HG13	1.96	0.47
1:D:227:ASN:ND2	1:D:232:CYS:HB3	2.21	0.47
1:D:243:LYS:HB2	1:D:265:TYR:CZ	2.49	0.47
1:F:193:MET:HA	1:F:210:HIS:NE2	2.30	0.47
1:C:245:ILE:HG22	1:C:247:VAL:HG23	1.95	0.47
1:D:213:ARG:O	1:D:217:LEU:HG	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:LYS:HE2	1:F:298:LYS:CA	2.30	0.47
1:E:309:PHE:CE1	1:E:313:ARG:NH2	2.83	0.47
1:F:196:PRO:HG3	1:F:210:HIS:HD1	1.80	0.47
1:C:245:ILE:CD1	1:C:262:ALA:HB2	2.44	0.47
1:D:228:VAL:CG1	1:D:290:ILE:HD12	2.44	0.47
1:F:245:ILE:CD1	1:F:262:ALA:HB2	2.45	0.47
1:D:245:ILE:O	1:D:247:VAL:HG23	2.15	0.47
1:A:233:PRO:HB2	1:A:235:HIS:CE1	2.50	0.47
1:B:212:ALA:HB3	1:C:215:ASP:HA	1.97	0.46
1:F:233:PRO:HB2	1:F:235:HIS:CE1	2.50	0.46
1:E:267:ASP:OD1	1:E:298:LYS:HD2	2.15	0.46
1:F:284:ILE:HG23	1:F:316:ILE:O	2.15	0.46
1:C:215:ASP:OD1	1:C:216:MET:N	2.45	0.46
1:E:209:TYR:HB2	1:F:219:ALA:HB2	1.97	0.46
1:D:267:ASP:OD1	1:D:298:LYS:HD2	2.14	0.46
1:E:256:SER:HA	1:E:259:PHE:CD2	2.50	0.46
1:D:193:MET:HA	1:D:210:HIS:NE2	2.30	0.46
1:B:309:PHE:CE1	1:B:313:ARG:NH2	2.84	0.46
1:C:228:VAL:HG11	1:C:290:ILE:HD12	1.96	0.46
1:F:298:LYS:CE	1:F:298:LYS:HA	2.32	0.46
1:F:245:ILE:HG22	1:F:245:ILE:O	2.16	0.46
1:E:250:ASN:HB3	1:E:252:LYS:N	2.31	0.46
1:B:307:PHE:O	1:B:311:LYS:HG2	2.16	0.46
1:A:215:ASP:OD1	1:A:216:MET:N	2.48	0.46
1:F:213:ARG:O	1:F:217:LEU:HG	2.16	0.46
1:C:267:ASP:OD1	1:C:298:LYS:HD2	2.15	0.45
1:A:250:ASN:HB3	1:A:252:LYS:N	2.30	0.45
1:A:228:VAL:CG1	1:A:290:ILE:HD12	2.45	0.45
1:E:213:ARG:O	1:E:217:LEU:HG	2.16	0.45
1:D:256:SER:HA	1:D:259:PHE:CD2	2.51	0.45
1:A:284:ILE:HG23	1:A:316:ILE:O	2.16	0.45
1:A:319:PRO:HD2	1:A:324:MET:HE1	1.98	0.45
1:D:253:ALA:HB3	1:D:323:PHE:HE2	1.81	0.45
1:A:245:ILE:CD1	1:A:262:ALA:HB2	2.46	0.45
1:D:319:PRO:HD2	1:D:324:MET:HE1	1.98	0.45
1:A:267:ASP:OD1	1:A:298:LYS:HD2	2.16	0.45
1:E:233:PRO:HB3	1:F:239:HIS:CD2	2.52	0.45
1:F:251:HIS:ND1	1:F:251:HIS:N	2.64	0.45
1:A:256:SER:HA	1:A:259:PHE:CD2	2.52	0.45
1:E:296:MET:O	1:E:300:ARG:CA	2.64	0.45
1:E:245:ILE:HD11	1:E:262:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:ASP:OD1	1:F:298:LYS:HD2	2.16	0.44
1:E:243:LYS:HB2	1:E:265:TYR:CZ	2.51	0.44
1:C:243:LYS:HB2	1:C:265:TYR:CZ	2.52	0.44
1:D:250:ASN:HB3	1:D:252:LYS:N	2.31	0.44
1:F:250:ASN:HB3	1:F:252:LYS:N	2.32	0.44
1:F:256:SER:HA	1:F:259:PHE:CD2	2.52	0.44
1:C:250:ASN:HB3	1:C:252:LYS:N	2.33	0.44
1:A:213:ARG:O	1:A:217:LEU:HG	2.18	0.44
1:B:267:ASP:OD1	1:B:298:LYS:HD2	2.17	0.44
1:C:193:MET:HA	1:C:210:HIS:NE2	2.33	0.44
1:E:251:HIS:ND1	1:E:251:HIS:N	2.64	0.44
1:B:250:ASN:HB3	1:B:252:LYS:N	2.32	0.44
1:F:228:VAL:CG1	1:F:290:ILE:HD12	2.47	0.44
1:B:245:ILE:O	1:B:245:ILE:HG22	2.17	0.44
1:B:328:LEU:O	1:B:331:GLU:HB3	2.17	0.44
1:D:307:PHE:O	1:D:311:LYS:HG2	2.17	0.44
1:A:243:LYS:HB2	1:A:265:TYR:CZ	2.53	0.44
1:B:284:ILE:HG23	1:B:316:ILE:O	2.17	0.43
1:F:317:ILE:HG22	1:F:319:PRO:HD3	2.00	0.43
1:F:302:ARG:HG3	1:F:302:ARG:HH11	1.83	0.43
1:D:285:SER:HB3	2:D:504:SO4:O2	2.17	0.43
1:C:298:LYS:CE	1:C:298:LYS:HA	2.33	0.43
1:A:251:HIS:ND1	1:A:251:HIS:N	2.65	0.43
1:C:249:ASP:OD1	1:C:285:SER:HB3	2.18	0.43
1:E:284:ILE:HG23	1:E:316:ILE:O	2.18	0.43
1:B:243:LYS:HB2	1:B:265:TYR:CZ	2.53	0.43
1:B:336:ALA:HB2	1:E:260:MET:CG	2.48	0.43
1:F:253:ALA:HB3	1:F:323:PHE:HE2	1.84	0.43
1:B:245:ILE:HD11	1:B:262:ALA:HB2	2.00	0.43
1:F:204:TYR:CE1	1:F:275:ARG:HD3	2.54	0.43
1:C:317:ILE:HG22	1:C:319:PRO:HD3	2.01	0.43
1:C:249:ASP:OD1	1:C:285:SER:CB	2.67	0.43
1:F:307:PHE:O	1:F:311:LYS:HG2	2.19	0.43
1:F:249:ASP:OD1	1:F:285:SER:HB3	2.19	0.43
1:F:243:LYS:HB2	1:F:265:TYR:CZ	2.54	0.42
1:C:247:VAL:HG12	1:C:248:GLU:N	2.34	0.42
1:A:204:TYR:CE1	1:A:275:ARG:HD3	2.54	0.42
1:C:253:ALA:HB3	1:C:323:PHE:HE2	1.84	0.42
1:B:269:VAL:HG11	1:B:276:VAL:HG22	2.02	0.42
1:D:310:VAL:CG1	1:D:317:ILE:HD11	2.39	0.42
1:D:320:ASN:OD1	1:D:322:SER:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:MET:O	1:C:300:ARG:CA	2.64	0.42
1:D:328:LEU:O	1:D:331:GLU:HB3	2.19	0.42
1:E:247:VAL:HG12	1:E:248:GLU:N	2.34	0.42
1:D:245:ILE:HD11	1:D:262:ALA:HB2	2.01	0.42
1:A:245:ILE:HG22	1:A:247:VAL:HG23	2.00	0.42
1:C:245:ILE:HA	1:C:246:PRO:HD2	1.84	0.42
1:D:249:ASP:OD1	1:D:285:SER:HB3	2.19	0.42
1:A:245:ILE:HG22	1:A:245:ILE:O	2.19	0.42
1:E:220:LEU:HD23	1:E:220:LEU:HA	1.85	0.42
1:C:307:PHE:O	1:C:311:LYS:HG2	2.19	0.42
1:A:314:ARG:HG2	1:A:316:ILE:HD13	2.01	0.42
1:D:249:ASP:OD1	1:D:285:SER:CB	2.68	0.42
1:E:253:ALA:HB3	1:E:323:PHE:HE2	1.84	0.42
1:E:307:PHE:O	1:E:311:LYS:HG2	2.20	0.42
1:F:228:VAL:HG11	1:F:290:ILE:HD12	2.00	0.42
1:B:228:VAL:CG1	1:B:290:ILE:HD12	2.50	0.42
1:A:328:LEU:O	1:A:331:GLU:HB3	2.20	0.42
1:F:247:VAL:HG12	1:F:248:GLU:N	2.35	0.42
1:E:249:ASP:OD1	1:E:285:SER:HB3	2.20	0.42
1:C:302:ARG:HG3	1:C:302:ARG:HH11	1.85	0.41
1:B:254:ASP:OD2	1:B:257:SER:HB3	2.20	0.41
1:C:319:PRO:HD2	1:C:324:MET:HE1	2.02	0.41
1:A:195:GLY:HA2	1:A:196:PRO:HD3	1.93	0.41
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.84	0.41
1:E:228:VAL:CG1	1:E:290:ILE:HD12	2.51	0.41
1:F:249:ASP:OD1	1:F:285:SER:CB	2.68	0.41
1:D:314:ARG:HG2	1:D:316:ILE:HD13	2.02	0.41
1:E:249:ASP:OD1	1:E:285:SER:CB	2.69	0.41
1:A:284:ILE:HG12	1:A:316:ILE:HG22	2.02	0.41
1:A:296:MET:O	1:A:300:ARG:CA	2.65	0.41
1:F:245:ILE:HA	1:F:246:PRO:HD2	1.84	0.41
1:B:247:VAL:HG12	1:B:248:GLU:N	2.36	0.41
1:E:204:TYR:CE1	1:E:275:ARG:HD3	2.56	0.41
1:F:215:ASP:OD1	1:F:216:MET:N	2.49	0.41
1:C:314:ARG:HG2	1:C:316:ILE:HD13	2.03	0.41
1:B:228:VAL:HG11	1:B:290:ILE:HD12	2.03	0.41
1:E:254:ASP:OD2	1:E:257:SER:HB3	2.20	0.41
1:C:297:MET:HA	1:C:334:VAL:HG11	2.03	0.41
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.86	0.41
1:E:298:LYS:HA	1:E:298:LYS:CE	2.30	0.41
1:C:227:ASN:ND2	1:C:232:CYS:HB3	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:THR:O	1:D:292:LEU:HB2	2.21	0.41
1:A:317:ILE:HG22	1:A:319:PRO:HD3	2.02	0.41
1:B:314:ARG:HG2	1:B:316:ILE:HD13	2.02	0.41
1:F:296:MET:O	1:F:300:ARG:CA	2.64	0.41
1:E:302:ARG:HH11	1:E:302:ARG:HG3	1.86	0.41
1:A:247:VAL:HG12	1:A:248:GLU:N	2.36	0.41
1:E:198:GLU:HG3	1:E:204:TYR:CZ	2.56	0.41
1:D:269:VAL:HG11	1:D:276:VAL:HG22	2.03	0.41
1:B:253:ALA:HB3	1:B:323:PHE:HE2	1.86	0.41
1:F:227:ASN:ND2	1:F:232:CYS:HB3	2.26	0.41
1:C:204:TYR:CE1	1:C:275:ARG:HD3	2.56	0.41
1:B:296:MET:O	1:B:300:ARG:CA	2.65	0.40
1:B:302:ARG:HH11	1:B:302:ARG:HG3	1.86	0.40
1:C:245:ILE:O	1:C:245:ILE:HG22	2.20	0.40
1:F:297:MET:HE3	1:F:334:VAL:HG13	2.03	0.40
1:E:328:LEU:O	1:E:331:GLU:HB3	2.21	0.40
1:B:298:LYS:CE	1:B:298:LYS:HA	2.31	0.40
1:E:233:PRO:HB3	1:F:239:HIS:HD2	1.87	0.40
1:F:323:PHE:N	1:F:323:PHE:CD2	2.90	0.40
1:A:304:GLU:CA	1:E:321:PHE:CD1	3.02	0.40
1:A:306:ALA:O	1:A:307:PHE:C	2.60	0.40
1:A:307:PHE:O	1:A:311:LYS:HG2	2.21	0.40
1:F:310:VAL:CG1	1:F:317:ILE:HD11	2.42	0.40
1:F:319:PRO:HD2	1:F:324:MET:HE1	2.03	0.40
1:B:251:HIS:N	1:B:251:HIS:ND1	2.66	0.40
1:E:245:ILE:HA	1:E:246:PRO:HD2	1.84	0.40
1:C:323:PHE:CD2	1:C:323:PHE:N	2.88	0.40
1:B:249:ASP:OD1	1:B:285:SER:HB3	2.21	0.40
1:A:323:PHE:CD2	1:A:323:PHE:N	2.89	0.40
1:D:316:ILE:CD1	1:D:316:ILE:N	2.78	0.40
1:E:212:ALA:HB3	1:F:215:ASP:HA	2.04	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	142/144 (99%)	122 (86%)	16 (11%)	4 (3%)	6	24
1	B	142/144 (99%)	122 (86%)	16 (11%)	4 (3%)	6	24
1	C	142/144 (99%)	122 (86%)	16 (11%)	4 (3%)	6	24
1	D	142/144 (99%)	123 (87%)	15 (11%)	4 (3%)	6	24
1	E	142/144 (99%)	123 (87%)	15 (11%)	4 (3%)	6	24
1	F	142/144 (99%)	123 (87%)	15 (11%)	4 (3%)	6	24
All	All	852/864 (99%)	735 (86%)	93 (11%)	24 (3%)	6	24

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	PRO
1	A	300	ARG
1	A	315	SER
1	B	246	PRO
1	B	300	ARG
1	B	315	SER
1	C	246	PRO
1	C	300	ARG
1	C	315	SER
1	D	300	ARG
1	D	315	SER
1	E	246	PRO
1	E	300	ARG
1	E	315	SER
1	F	246	PRO
1	F	300	ARG
1	F	315	SER
1	D	246	PRO
1	B	228	VAL
1	C	228	VAL
1	D	228	VAL
1	A	228	VAL
1	E	228	VAL
1	F	228	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/123 (100%)	119 (97%)	4 (3%)	45	80
1	B	123/123 (100%)	119 (97%)	4 (3%)	45	80
1	C	123/123 (100%)	119 (97%)	4 (3%)	45	80
1	D	123/123 (100%)	119 (97%)	4 (3%)	45	80
1	E	123/123 (100%)	119 (97%)	4 (3%)	45	80
1	F	123/123 (100%)	119 (97%)	4 (3%)	45	80
All	All	738/738 (100%)	714 (97%)	24 (3%)	45	80

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	MET
1	A	231	ASP
1	A	297	MET
1	A	315	SER
1	B	193	MET
1	B	231	ASP
1	B	297	MET
1	B	315	SER
1	C	193	MET
1	C	231	ASP
1	C	297	MET
1	C	315	SER
1	D	193	MET
1	D	231	ASP
1	D	297	MET
1	D	315	SER
1	E	193	MET
1	E	231	ASP
1	E	297	MET
1	E	315	SER
1	F	193	MET
1	F	231	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	297	MET
1	F	315	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	235	HIS
1	A	279	HIS
1	A	281	GLN
1	A	312	GLN
1	A	333	GLN
1	B	234	ASN
1	B	279	HIS
1	B	281	GLN
1	B	312	GLN
1	C	234	ASN
1	C	235	HIS
1	C	250	ASN
1	C	279	HIS
1	C	281	GLN
1	C	312	GLN
1	D	234	ASN
1	D	235	HIS
1	D	279	HIS
1	D	281	GLN
1	D	312	GLN
1	E	234	ASN
1	E	279	HIS
1	E	281	GLN
1	E	312	GLN
1	F	234	ASN
1	F	235	HIS
1	F	279	HIS
1	F	281	GLN
1	F	312	GLN

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)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	501	-	4,4,4	0.10	0	6,6,6	0.12	0
2	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	B	502	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	C	503	-	4,4,4	0.18	0	6,6,6	0.07	0
2	SO4	C	509	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	D	504	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	D	508	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	E	505	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	F	506	-	4,4,4	0.18	0	6,6,6	0.11	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	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	509	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	508	-	-	0/0/0/0	0/0/0/0
2	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	SO4	F	506	-	-	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	504	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	144/144 (100%)	1.04	12 (8%) 14 9	43, 71, 89, 95	0
1	B	144/144 (100%)	0.72	6 (4%) 40 33	43, 71, 89, 95	0
1	C	144/144 (100%)	0.73	16 (11%) 7 4	43, 71, 89, 95	0
1	D	144/144 (100%)	1.01	24 (16%) 2 1	43, 71, 89, 95	0
1	E	144/144 (100%)	0.75	10 (6%) 20 14	43, 71, 89, 95	0
1	F	144/144 (100%)	0.77	14 (9%) 10 6	43, 71, 89, 95	0
All	All	864/864 (100%)	0.84	82 (9%) 10 6	43, 71, 90, 95	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	VAL	6.0
1	B	336	ALA	5.3
1	C	336	ALA	4.1
1	D	255	ILE	4.0
1	C	330	PHE	4.0
1	D	330	PHE	3.9
1	E	336	ALA	3.6
1	C	334	VAL	3.5
1	C	301	VAL	3.5
1	D	226	LEU	3.4
1	D	304	GLU	3.4
1	F	321	PHE	3.3
1	C	193	MET	3.3
1	B	303	LEU	3.2
1	C	228	VAL	3.2
1	C	321	PHE	3.1
1	D	324	MET	3.1
1	D	292	LEU	3.0
1	F	193	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	335	LEU	3.0
1	D	321	PHE	3.0
1	D	245	ILE	2.9
1	B	255	ILE	2.9
1	D	228	VAL	2.9
1	F	336	ALA	2.9
1	D	301	VAL	2.8
1	E	193	MET	2.8
1	B	335	LEU	2.8
1	F	323	PHE	2.8
1	A	228	VAL	2.8
1	F	273	ARG	2.8
1	E	250	ASN	2.7
1	E	324	MET	2.7
1	E	334	VAL	2.7
1	D	300	ARG	2.7
1	B	334	VAL	2.7
1	C	324	MET	2.7
1	D	332	SER	2.7
1	D	336	ALA	2.6
1	C	289	THR	2.6
1	D	302	ARG	2.6
1	F	302	ARG	2.5
1	F	255	ILE	2.5
1	A	227	ASN	2.5
1	A	247	VAL	2.5
1	A	290	ILE	2.5
1	C	287	SER	2.4
1	F	251	HIS	2.4
1	F	330	PHE	2.4
1	E	228	VAL	2.4
1	D	296	MET	2.4
1	E	247	VAL	2.4
1	D	297	MET	2.4
1	A	226	LEU	2.3
1	D	252	LYS	2.3
1	C	327	LEU	2.3
1	D	277	LEU	2.3
1	C	255	ILE	2.3
1	F	335	LEU	2.3
1	A	307	PHE	2.3
1	E	255	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	328	LEU	2.3
1	A	293	ALA	2.2
1	F	322	SER	2.2
1	A	255	ILE	2.2
1	C	247	VAL	2.2
1	B	253	ALA	2.2
1	A	317	ILE	2.1
1	C	290	ILE	2.1
1	F	300	ARG	2.1
1	E	226	LEU	2.1
1	E	283	GLY	2.1
1	F	241	GLN	2.1
1	A	217	LEU	2.1
1	D	251	HIS	2.1
1	C	300	ARG	2.1
1	A	284	ILE	2.0
1	C	292	LEU	2.0
1	D	329	GLN	2.0
1	D	225	LEU	2.0
1	F	228	VAL	2.0
1	A	222	ILE	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	B	502	5/5	0.96	0.29	0.98	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	C	509	5/5	0.98	0.24	-0.19	58,58,58,58	0
2	SO4	C	503	5/5	0.98	0.20	-0.58	77,77,77,77	0
2	SO4	D	504	5/5	0.89	0.19	-0.86	95,95,95,95	0
2	SO4	F	506	5/5	0.95	0.16	-1.05	71,71,71,71	0
2	SO4	E	505	5/5	0.97	0.16	-1.50	43,43,43,43	0
2	SO4	A	501	5/5	0.98	0.21	-1.59	36,36,36,36	0
2	SO4	D	508	5/5	0.99	0.30	-	67,67,67,67	5
2	SO4	A	507	5/5	0.98	0.32	-	76,76,76,76	5

6.5 Other polymers (i)

There are no such residues in this entry.