Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:53 PM GMT

PDB ID	:	3VB0
Title	:	Crystal structure of 2,2',3-trihydroxybiphenyl 1,2-dioxygenase from dibenzofuran-degrading Sphingomonas wittichii strain RW1
Authors	:	Koksal, M.; Kumar, P.; Bolin, J.T.
Deposited on	:	2011-12-30
Resolution	:	2.10 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:

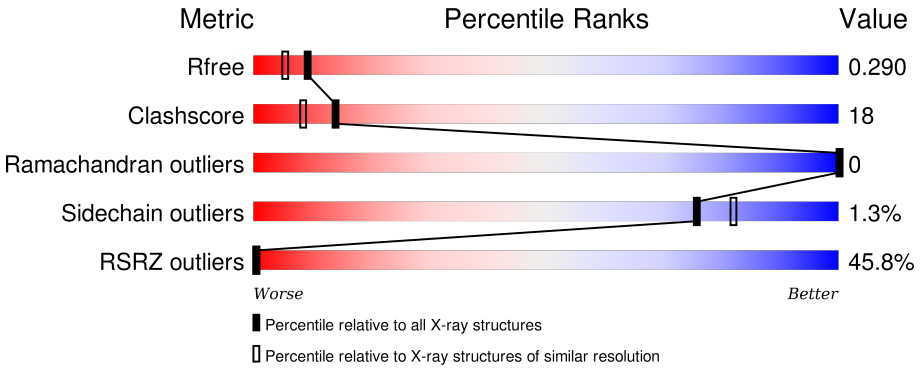
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	294	13% 90% 8% ·
1	B	294	17% 88% 10% ·
1	C	294	71% 58% 39% ··
1	D	294	79% 61% 36% ··

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P6G	B	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9162 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.

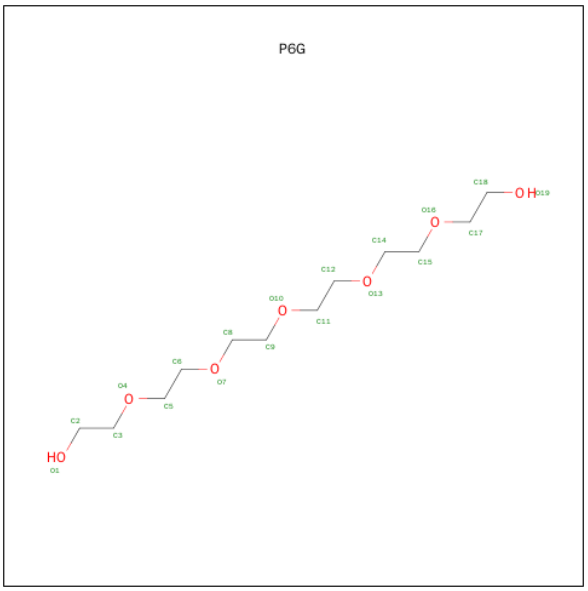
- Molecule 1 is a protein called Glyoxalase/bleomycin resistance protein/dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	B	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	C	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	D	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

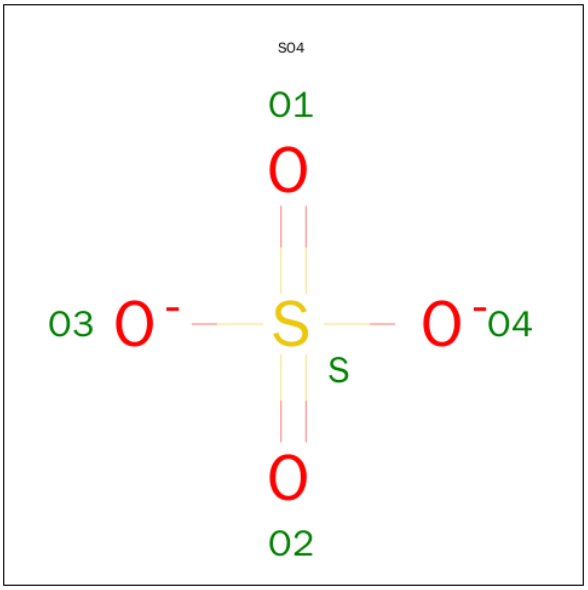
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

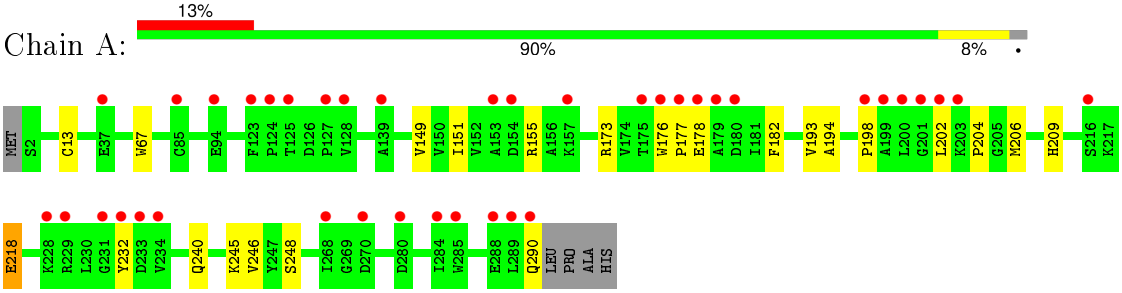
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	80	Total O 80 80	0	0
5	C	1	Total O 1 1	0	0

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.

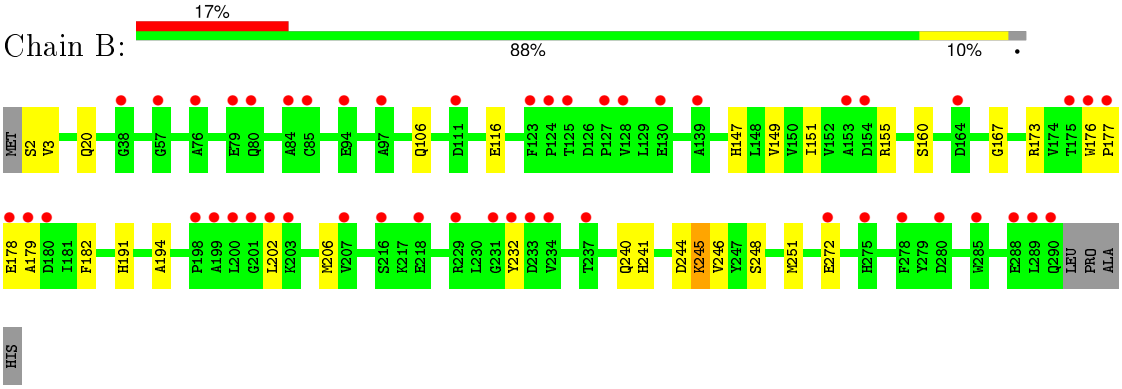
- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

Chain A:



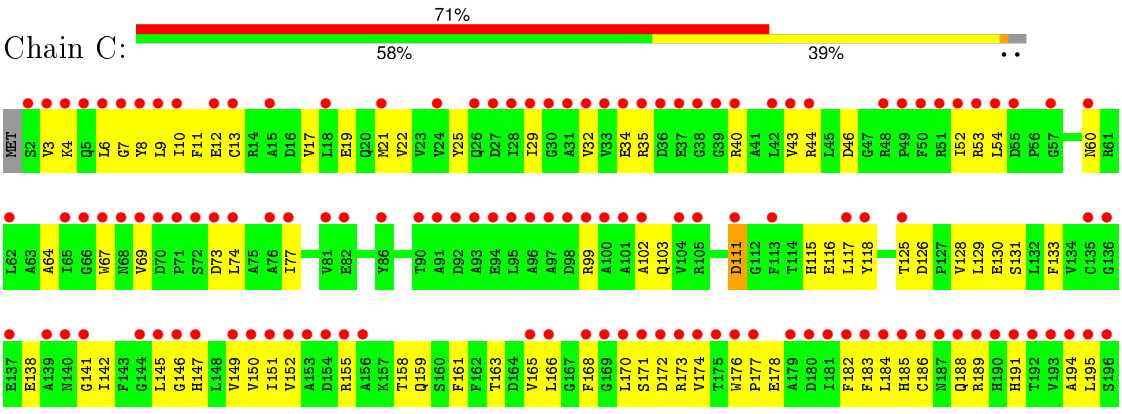
- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

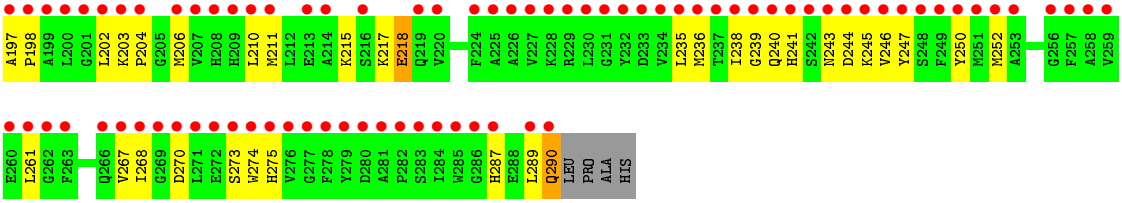
Chain B:



- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

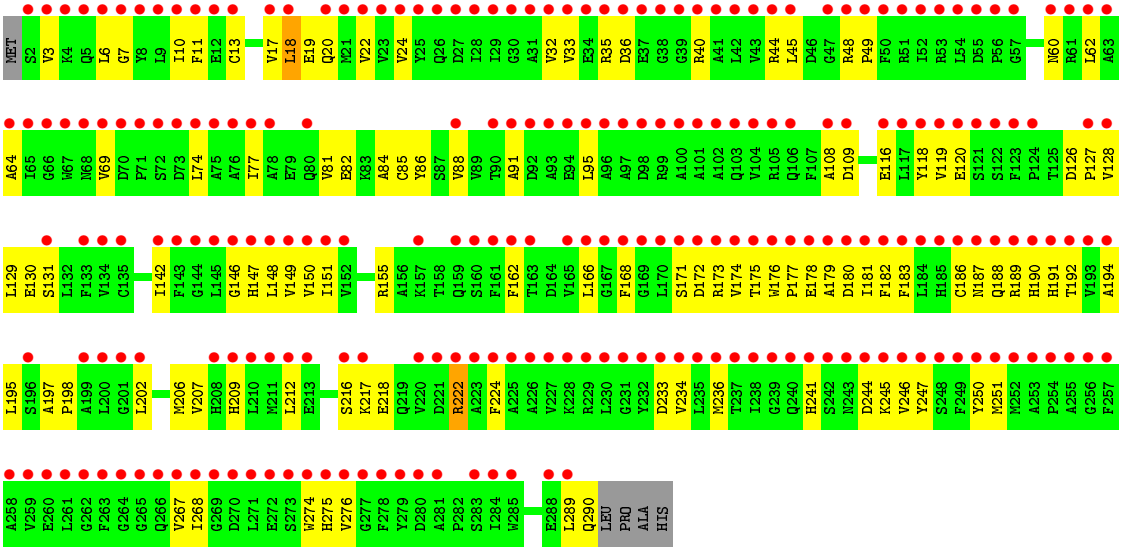
Chain C:





• Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.59Å 131.59Å 103.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.10 34.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (92.85-2.10) 97.9 (34.54-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.289 0.254 , 0.290	Depositor DCC
R_{free} test set	2640 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	13 of 52453 reflections (0.025%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9162	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.87 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.9012e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FE2, SO4, P6G

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	0.55	1/2291 (0.0%)	0.61	0/3111
1	B	0.56	0/2291	0.61	0/3111
1	C	0.33	0/2291	0.47	0/3111
1	D	0.33	0/2291	0.48	0/3111
All	All	0.46	1/9164 (0.0%)	0.55	0/12444

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	CYS	CB-SG	-5.64	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2173	26	0
1	B	2238	0	2173	33	0
1	C	2238	0	2173	135	0
1	D	2238	0	2173	140	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	26	2	0
3	B	19	0	26	9	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	77	0	0	0	0
5	B	80	0	0	0	0
5	C	1	0	0	0	0
All	All	9162	0	8744	325	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 18.

All (325) 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:C:168:PHE:CD1	1:C:186:CYS:HB3	1.20	1.63
1:C:217:LYS:NZ	1:C:247:TYR:CZ	1.76	1.53
1:C:168:PHE:HE1	1:C:186:CYS:SG	1.32	1.52
1:D:176:TRP:NE1	1:D:178:GLU:HG2	1.24	1.51
1:D:176:TRP:NE1	1:D:178:GLU:CG	1.81	1.42
1:D:176:TRP:HE1	1:D:178:GLU:CG	1.33	1.32
1:C:168:PHE:CE1	1:C:186:CYS:SG	2.20	1.32
1:D:217:LYS:NZ	1:D:247:TYR:CZ	1.98	1.30
1:C:168:PHE:CE1	1:C:186:CYS:HB3	1.66	1.29
1:C:168:PHE:CE1	1:C:186:CYS:CB	2.16	1.29
1:C:168:PHE:CD1	1:C:186:CYS:CB	2.14	1.27
1:C:9:LEU:CD1	1:C:210:LEU:HD11	1.68	1.24
1:D:176:TRP:CD1	1:D:178:GLU:HG2	1.72	1.23
1:D:176:TRP:HE1	1:D:178:GLU:CD	1.46	1.18
1:D:86:TYR:CE1	1:D:109:ASP:HA	1.80	1.16
1:C:13:CYS:HA	1:C:60:ASN:OD1	1.44	1.14
1:D:126:ASP:C	1:D:130:GLU:OE1	1.89	1.11
1:C:203:LYS:O	1:C:206:MET:HG3	1.49	1.11
1:C:176:TRP:NE1	1:C:178:GLU:HG2	1.69	1.08
1:D:202:LEU:HD22	1:D:206:MET:HE2	1.36	1.07
1:C:149:VAL:HG22	1:C:194:ALA:HB3	1.37	1.05
1:A:176:TRP:NE1	1:A:178:GLU:CG	2.19	1.05
1:C:236:MET:CE	1:C:287:HIS:HB3	1.86	1.04
1:C:29:ILE:HD12	1:C:261:LEU:HD13	1.32	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:NE1	1:A:178:GLU:HG2	1.73	1.04
1:D:155:ARG:HD2	1:D:182:PHE:CD2	1.93	1.03
1:C:217:LYS:NZ	1:C:247:TYR:OH	1.93	1.00
1:C:9:LEU:HD13	1:C:210:LEU:HD11	1.41	1.00
1:D:202:LEU:HD22	1:D:206:MET:CE	1.93	0.97
1:C:236:MET:HE3	1:C:287:HIS:HB3	1.43	0.97
1:D:188:GLN:HG3	1:D:268:ILE:O	1.65	0.96
1:A:176:TRP:HE1	1:A:178:GLU:CD	1.70	0.95
1:A:176:TRP:CD1	1:A:178:GLU:HG2	2.01	0.94
1:D:45:LEU:HD11	1:D:212:LEU:HD22	1.47	0.94
1:D:217:LYS:NZ	1:D:247:TYR:CE1	2.26	0.94
1:D:155:ARG:CD	1:D:182:PHE:CD2	2.51	0.93
1:C:19:GLU:OE1	1:C:35:ARG:NH2	2.02	0.93
1:C:217:LYS:NZ	1:C:247:TYR:CE1	2.24	0.92
1:D:45:LEU:HD11	1:D:212:LEU:CD2	2.00	0.92
1:D:244:ASP:OD2	1:D:246:VAL:HG22	1.69	0.91
1:D:173:ARG:HD2	1:D:182:PHE:CE1	2.05	0.91
1:D:36:ASP:OD2	1:D:40:ARG:HD2	1.70	0.91
1:D:82:GLU:OE1	1:D:88:VAL:N	2.02	0.91
1:C:176:TRP:NE1	1:C:178:GLU:CG	2.35	0.89
1:D:244:ASP:CG	1:D:246:VAL:HG22	1.92	0.89
1:B:251:MET:HE3	3:B:302:P6G:H62	1.55	0.89
1:C:19:GLU:CD	1:C:35:ARG:HH22	1.74	0.88
1:C:176:TRP:CD1	1:C:178:GLU:HG2	2.08	0.88
1:D:244:ASP:OD2	1:D:246:VAL:CG2	2.23	0.87
1:C:176:TRP:HE1	1:C:178:GLU:CG	1.87	0.86
1:D:45:LEU:CD1	1:D:212:LEU:HD22	2.05	0.86
1:C:168:PHE:HD1	1:C:186:CYS:CB	1.70	0.86
1:D:86:TYR:HE1	1:D:109:ASP:HA	1.39	0.86
1:C:170:LEU:HA	1:C:184:LEU:HD23	1.57	0.86
1:C:203:LYS:N	1:C:206:MET:SD	2.48	0.85
1:D:126:ASP:O	1:D:130:GLU:OE1	1.97	0.83
1:C:244:ASP:CG	1:C:246:VAL:HG23	1.99	0.82
1:D:17:VAL:HA	1:D:20:GLN:OE1	1.80	0.81
1:D:218:GLU:O	1:D:222:ARG:HG2	1.81	0.81
1:D:3:VAL:HG21	1:D:168:PHE:CE2	2.17	0.80
1:C:236:MET:HE2	1:C:287:HIS:HB3	1.63	0.79
1:C:13:CYS:CA	1:C:60:ASN:OD1	2.28	0.79
1:A:176:TRP:HE1	1:A:178:GLU:CG	1.90	0.79
1:C:241:HIS:HB2	1:C:244:ASP:OD1	1.83	0.79
1:B:251:MET:HE3	3:B:302:P6G:C6	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:OD2	1:C:246:VAL:CG2	2.32	0.77
1:D:149:VAL:HG21	1:D:209:HIS:CE1	2.21	0.76
1:C:168:PHE:HE1	1:C:186:CYS:CB	1.75	0.75
1:D:176:TRP:NE1	1:D:178:GLU:HG3	1.95	0.75
1:B:173:ARG:NH1	1:C:273:SER:OG	2.20	0.75
1:C:244:ASP:OD2	1:C:246:VAL:HG23	1.86	0.74
1:C:236:MET:CE	1:C:287:HIS:CB	2.66	0.74
1:D:149:VAL:HG22	1:D:194:ALA:HB3	1.69	0.73
1:D:173:ARG:HH11	1:D:182:PHE:HZ	1.30	0.72
1:B:173:ARG:HH12	1:C:270:ASP:CG	1.93	0.72
1:D:218:GLU:O	1:D:222:ARG:CG	2.38	0.72
1:B:173:ARG:NH1	1:C:270:ASP:CB	2.52	0.72
1:C:149:VAL:CG2	1:C:194:ALA:HB3	2.17	0.71
1:C:159:GLN:O	1:C:163:THR:OG1	2.04	0.71
1:D:176:TRP:CE2	1:D:178:GLU:CG	2.72	0.70
1:D:24:VAL:HG13	1:D:251:MET:HE1	1.73	0.70
1:B:173:ARG:NH1	1:C:270:ASP:HB3	2.07	0.70
1:D:217:LYS:NZ	1:D:247:TYR:OH	2.25	0.70
1:D:174:VAL:HG23	1:D:183:PHE:CE2	2.26	0.69
1:C:236:MET:HE2	1:C:287:HIS:CB	2.22	0.69
1:D:24:VAL:HG13	1:D:251:MET:CE	2.23	0.69
1:D:155:ARG:CD	1:D:182:PHE:CE2	2.76	0.68
1:C:9:LEU:HD13	1:C:210:LEU:CD1	2.22	0.68
1:C:126:ASP:O	1:C:130:GLU:HG3	1.94	0.68
1:C:29:ILE:HD13	1:C:261:LEU:HD22	1.74	0.68
1:C:32:VAL:HG23	1:C:129:LEU:HD13	1.74	0.68
1:A:232:TYR:CZ	3:A:302:P6G:H31	2.29	0.68
1:C:9:LEU:HD12	1:C:210:LEU:HD11	1.71	0.67
1:B:251:MET:CE	3:B:302:P6G:H62	2.23	0.67
1:C:102:ALA:O	1:C:103:GLN:HG3	1.95	0.67
1:D:173:ARG:NH1	1:D:182:PHE:CZ	2.59	0.66
1:D:11:PHE:CE1	1:D:62:LEU:HD13	2.30	0.66
1:D:176:TRP:NE1	1:D:178:GLU:CD	2.31	0.66
1:C:149:VAL:HG22	1:C:194:ALA:CB	2.20	0.65
1:D:36:ASP:OD2	1:D:40:ARG:CD	2.44	0.65
1:C:161:PHE:CD1	1:C:165:VAL:HG21	2.32	0.65
1:D:176:TRP:CZ2	1:D:179:ALA:HB3	2.33	0.64
1:D:128:VAL:O	1:D:131:SER:OG	2.13	0.64
1:C:176:TRP:HB2	1:C:177:PRO:HD2	1.80	0.64
1:C:151:ILE:HG13	1:C:202:LEU:HB3	1.80	0.64
1:D:176:TRP:CE2	1:D:178:GLU:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:HD1	1:C:186:CYS:HB3	0.84	0.63
1:B:232:TYR:CZ	3:B:302:P6G:H31	2.33	0.63
1:B:149:VAL:HG22	1:B:194:ALA:HB3	1.80	0.63
1:D:173:ARG:HD2	1:D:182:PHE:CZ	2.33	0.63
1:D:197:ALA:HB1	1:D:198:PRO:HD2	1.80	0.63
1:D:241:HIS:HB2	1:D:244:ASP:OD1	1.99	0.62
1:C:172:ASP:OD2	1:C:243:ASN:HB2	1.99	0.62
1:D:3:VAL:HG11	1:D:166:LEU:HD22	1.81	0.62
1:C:173:ARG:HD2	1:C:182:PHE:CE1	2.35	0.61
1:C:133:PHE:O	1:C:215:LYS:HE3	2.00	0.61
1:C:176:TRP:HE1	1:C:178:GLU:CD	2.04	0.61
1:C:3:VAL:HG23	1:C:166:LEU:O	2.01	0.61
1:D:17:VAL:HG11	1:D:60:ASN:OD1	2.00	0.61
1:D:162:PHE:HD2	1:D:168:PHE:CD2	2.19	0.60
1:C:67:TRP:HB2	1:C:117:LEU:HD23	1.82	0.60
1:B:176:TRP:NE1	1:B:178:GLU:HG2	2.17	0.60
1:C:176:TRP:HB2	1:C:177:PRO:CD	2.32	0.60
1:D:202:LEU:HD22	1:D:206:MET:HE1	1.83	0.60
1:D:216:SER:HB2	1:D:218:GLU:OE1	2.01	0.60
1:D:48:ARG:HG2	1:D:49:PRO:HD2	1.84	0.59
1:D:176:TRP:HB2	1:D:177:PRO:HD2	1.85	0.59
1:D:176:TRP:CH2	1:D:179:ALA:HB3	2.37	0.59
1:A:202:LEU:HD22	1:A:206:MET:CE	2.32	0.59
1:D:86:TYR:CD1	1:D:108:ALA:O	2.56	0.58
1:D:175:THR:OG1	1:D:180:ASP:OD1	2.21	0.58
1:C:10:ILE:HD12	1:C:64:ALA:HB3	1.84	0.58
1:D:74:LEU:HD22	1:D:119:VAL:HG23	1.85	0.58
1:D:176:TRP:HB2	1:D:177:PRO:CD	2.34	0.58
1:C:73:ASP:HB3	1:C:77:ILE:HD11	1.86	0.58
1:A:202:LEU:HD22	1:A:206:MET:HE2	1.84	0.58
1:C:146:GLY:HA2	1:C:189:ARG:CZ	2.33	0.58
1:D:81:VAL:HG12	1:D:86:TYR:HB2	1.85	0.57
1:C:3:VAL:CG1	1:C:67:TRP:HB3	2.33	0.57
1:B:173:ARG:NH1	1:C:270:ASP:CG	2.57	0.57
1:C:176:TRP:HE1	1:C:178:GLU:HG2	1.49	0.57
1:C:29:ILE:HD11	1:C:261:LEU:HB2	1.85	0.57
1:D:3:VAL:CG1	1:D:166:LEU:HD22	2.33	0.57
1:D:127:PRO:N	1:D:130:GLU:OE1	2.37	0.57
1:D:289:LEU:O	1:D:290:GLN:HB2	2.05	0.57
1:C:9:LEU:HD11	1:C:210:LEU:HD11	1.79	0.57
1:C:244:ASP:OD2	1:C:246:VAL:HG21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD21	1:C:9:LEU:HD21	1.85	0.57
1:B:160:SER:HB2	1:C:275:HIS:HE1	1.68	0.57
1:D:202:LEU:CD2	1:D:206:MET:CE	2.77	0.56
1:D:244:ASP:OD2	1:D:246:VAL:HG21	2.03	0.56
1:D:3:VAL:HA	1:D:69:VAL:HG12	1.87	0.56
1:A:149:VAL:HG22	1:A:194:ALA:HB3	1.86	0.56
1:B:232:TYR:CG	3:B:302:P6G:H51	2.41	0.56
1:D:128:VAL:HG23	1:D:129:LEU:N	2.21	0.56
1:C:155:ARG:HD2	1:C:182:PHE:CD2	2.40	0.56
1:C:29:ILE:CD1	1:C:261:LEU:HB2	2.36	0.56
1:A:173:ARG:HH11	1:A:182:PHE:HZ	1.53	0.56
1:D:151:ILE:HD11	1:D:202:LEU:HD12	1.86	0.56
1:D:155:ARG:NE	1:D:182:PHE:CE2	2.75	0.55
1:C:197:ALA:HB1	1:C:198:PRO:HD2	1.88	0.55
1:D:13:CYS:HB2	1:D:18:LEU:HD12	1.88	0.55
1:D:10:ILE:HD12	1:D:64:ALA:HB3	1.88	0.55
1:C:268:ILE:HD12	1:C:274:TRP:CD2	2.42	0.55
1:D:22:VAL:HG21	1:D:35:ARG:HH21	1.73	0.54
1:B:202:LEU:HD22	1:B:206:MET:CE	2.38	0.54
1:D:173:ARG:NH1	1:D:182:PHE:HZ	1.97	0.54
1:D:84:ALA:O	1:D:85:CYS:HB2	2.07	0.54
1:D:155:ARG:CZ	1:D:182:PHE:CZ	2.91	0.54
1:B:176:TRP:HB2	1:B:177:PRO:CD	2.37	0.54
1:B:246:VAL:HG12	1:B:248:SER:HB3	1.89	0.54
1:D:148:LEU:HD11	1:D:207:VAL:HG13	1.90	0.54
1:C:17:VAL:HG21	1:C:60:ASN:ND2	2.22	0.53
1:D:155:ARG:CZ	1:D:182:PHE:CE2	2.92	0.53
1:B:151:ILE:HG13	1:B:202:LEU:HB3	1.90	0.53
1:C:4:LYS:HE2	1:C:142:ILE:HD12	1.91	0.53
1:C:69:VAL:HG21	1:C:74:LEU:HD13	1.90	0.53
1:D:244:ASP:OD1	1:D:246:VAL:HG22	2.08	0.53
1:B:202:LEU:HD22	1:B:206:MET:HE2	1.90	0.53
1:D:3:VAL:CG2	1:D:168:PHE:CE2	2.90	0.53
1:D:176:TRP:HH2	1:D:181:ILE:HD12	1.74	0.53
1:D:151:ILE:HG13	1:D:202:LEU:CD1	2.40	0.52
1:D:176:TRP:CH2	1:D:181:ILE:HD12	2.45	0.52
1:D:3:VAL:HG21	1:D:168:PHE:CZ	2.44	0.52
1:D:173:ARG:CZ	1:D:180:ASP:OD1	2.57	0.52
1:C:21:MET:HE2	1:C:25:TYR:HE2	1.75	0.52
1:C:17:VAL:HG21	1:C:60:ASN:HD21	1.74	0.52
1:D:174:VAL:HG23	1:D:183:PHE:HE2	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ARG:HD3	1:D:182:PHE:CE2	2.44	0.51
1:C:236:MET:CE	1:C:287:HIS:CG	2.93	0.51
1:D:241:HIS:CB	1:D:244:ASP:OD1	2.58	0.51
1:D:174:VAL:CG2	1:D:183:PHE:CE2	2.94	0.51
1:D:149:VAL:CG2	1:D:209:HIS:CE1	2.93	0.51
1:C:29:ILE:CD1	1:C:261:LEU:HD13	2.23	0.51
1:C:197:ALA:HB1	1:C:198:PRO:CD	2.40	0.51
1:D:202:LEU:CD2	1:D:206:MET:HE1	2.40	0.51
1:D:45:LEU:HD11	1:D:212:LEU:HD21	1.88	0.51
1:D:126:ASP:N	1:D:130:GLU:OE1	2.44	0.51
1:C:147:HIS:HB3	1:C:191:HIS:O	2.11	0.51
1:B:160:SER:HB2	1:C:275:HIS:CE1	2.45	0.50
1:D:45:LEU:CD1	1:D:212:LEU:CD2	2.75	0.50
1:A:149:VAL:HG21	1:A:209:HIS:CE1	2.46	0.50
1:C:155:ARG:CD	1:C:182:PHE:CD2	2.95	0.50
1:B:251:MET:CE	3:B:302:P6G:C6	2.85	0.50
1:D:32:VAL:HG23	1:D:129:LEU:CD1	2.42	0.50
1:D:126:ASP:H	1:D:130:GLU:CD	2.15	0.50
1:D:224:PHE:HE1	1:D:234:VAL:HG11	1.78	0.49
1:D:7:GLY:HA3	1:D:118:TYR:OH	2.13	0.49
1:A:176:TRP:NE1	1:A:178:GLU:HG3	2.23	0.49
1:C:111:ASP:OD1	1:C:152:VAL:HA	2.12	0.49
1:C:236:MET:HB2	1:C:250:TYR:HB2	1.95	0.49
1:D:151:ILE:HG13	1:D:202:LEU:HD13	1.95	0.48
1:C:7:GLY:HA3	1:C:118:TYR:OH	2.13	0.48
1:A:176:TRP:CE2	1:A:178:GLU:CG	2.94	0.48
1:D:45:LEU:HD13	1:D:212:LEU:HD22	1.91	0.48
1:D:147:HIS:HB3	1:D:191:HIS:O	2.13	0.48
1:C:217:LYS:HG3	1:C:247:TYR:CE2	2.48	0.48
1:D:218:GLU:O	1:D:222:ARG:HG3	2.12	0.48
1:C:73:ASP:O	1:C:77:ILE:HG13	2.13	0.48
1:D:148:LEU:CD1	1:D:207:VAL:HG13	2.43	0.48
1:C:12:GLU:O	1:C:60:ASN:HA	2.14	0.48
1:C:3:VAL:HG13	1:C:67:TRP:HB3	1.96	0.47
1:C:203:LYS:O	1:C:206:MET:CG	2.41	0.47
1:C:128:VAL:O	1:C:131:SER:OG	2.26	0.47
1:D:91:ALA:HB1	1:D:95:LEU:HB3	1.96	0.47
1:A:240:GLN:HA	1:A:246:VAL:O	2.14	0.47
1:A:176:TRP:CE2	1:A:178:GLU:HG3	2.49	0.47
1:C:29:ILE:HD12	1:C:261:LEU:CD1	2.24	0.47
1:C:241:HIS:CB	1:C:244:ASP:OD1	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:MET:HE1	3:B:302:P6G:H52	1.97	0.47
1:C:289:LEU:O	1:C:290:GLN:HB2	2.13	0.47
1:C:240:GLN:HA	1:C:246:VAL:O	2.15	0.47
1:D:44:ARG:NH2	1:D:126:ASP:OD2	2.45	0.47
1:D:162:PHE:CD2	1:D:168:PHE:CE2	3.03	0.47
1:B:106:GLN:HG3	1:B:116:GLU:HG2	1.97	0.47
1:B:155:ARG:HD3	1:B:182:PHE:CD2	2.51	0.46
1:C:203:LYS:HB3	1:C:204:PRO:HD2	1.97	0.46
1:C:29:ILE:CD1	1:C:261:LEU:HD22	2.44	0.46
1:D:48:ARG:CG	1:D:49:PRO:HD2	2.45	0.46
1:D:77:ILE:O	1:D:81:VAL:HG23	2.15	0.46
1:B:173:ARG:HH12	1:C:270:ASP:CB	2.26	0.46
1:C:11:PHE:HB2	1:C:54:LEU:HD23	1.97	0.46
1:B:232:TYR:CD2	3:B:302:P6G:H51	2.51	0.46
1:C:158:THR:HG22	1:C:195:LEU:HD11	1.97	0.46
1:C:171:SER:OG	1:C:185:HIS:ND1	2.30	0.46
1:D:22:VAL:HG13	1:D:33:VAL:HG11	1.96	0.46
1:D:168:PHE:CD1	1:D:186:CYS:HB3	2.50	0.46
1:A:155:ARG:HD3	1:A:182:PHE:CD2	2.51	0.46
1:D:86:TYR:CZ	1:D:109:ASP:HA	2.46	0.46
1:D:151:ILE:CD1	1:D:202:LEU:HD12	2.46	0.46
1:B:244:ASP:O	1:B:245:LYS:HB2	2.15	0.46
1:B:176:TRP:CH2	1:B:179:ALA:HB3	2.51	0.45
1:D:19:GLU:OE2	1:D:35:ARG:NH2	2.48	0.45
1:C:239:GLY:C	1:C:287:HIS:CE1	2.89	0.45
1:A:218:GLU:CD	1:A:218:GLU:H	2.18	0.45
1:C:3:VAL:HG11	1:C:67:TRP:HB3	1.98	0.45
1:C:10:ILE:HD11	1:C:99:ARG:CD	2.47	0.45
1:D:6:LEU:HB2	1:D:192:THR:CG2	2.47	0.45
1:C:217:LYS:HG3	1:C:247:TYR:CD2	2.52	0.44
1:D:35:ARG:HD3	1:D:40:ARG:O	2.17	0.44
1:B:20:GLN:HB3	3:B:302:P6G:H22	1.98	0.44
1:D:162:PHE:CD2	1:D:168:PHE:CD2	3.03	0.44
1:C:235:LEU:HD22	1:C:252:MET:HE2	1.99	0.44
1:D:19:GLU:CD	1:D:35:ARG:NH2	2.71	0.44
1:D:11:PHE:CZ	1:D:62:LEU:HD13	2.52	0.44
1:A:151:ILE:HG13	1:A:202:LEU:HB3	1.99	0.44
1:C:238:ILE:HG21	1:C:247:TYR:CZ	2.53	0.44
1:C:268:ILE:HD12	1:C:274:TRP:CE2	2.53	0.44
1:D:244:ASP:O	1:D:245:LYS:HB2	2.18	0.44
1:C:32:VAL:CG2	1:C:129:LEU:HD13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD23	1:C:211:MET:H	1.83	0.44
1:C:150:VAL:HG23	1:C:195:LEU:HD23	2.00	0.44
1:B:241:HIS:HB2	1:B:244:ASP:OD1	2.18	0.44
1:B:272:GLU:O	1:C:245:LYS:HE3	2.18	0.44
1:D:48:ARG:HE	1:D:120:GLU:CD	2.19	0.43
1:D:275:HIS:HD2	1:D:276:VAL:O	2.01	0.43
1:C:151:ILE:HD11	1:C:202:LEU:CD1	2.48	0.43
1:D:236:MET:HB2	1:D:250:TYR:HB2	2.00	0.43
1:A:176:TRP:HB2	1:A:177:PRO:CD	2.49	0.43
1:C:161:PHE:O	1:C:165:VAL:HB	2.18	0.43
1:D:146:GLY:HA2	1:D:189:ARG:CZ	2.49	0.43
1:D:32:VAL:HG23	1:D:129:LEU:HD11	2.01	0.43
1:C:141:GLY:HA3	1:C:188:GLN:HG2	2.01	0.43
1:C:22:VAL:HG21	1:C:35:ARG:NH2	2.34	0.42
1:B:2:SER:HB2	1:B:167:GLY:HA3	2.01	0.42
1:D:17:VAL:HG21	1:D:60:ASN:HD21	1.83	0.42
1:D:91:ALA:CB	1:D:95:LEU:HD23	2.48	0.42
1:A:198:PRO:HG3	1:A:204:PRO:HD3	2.01	0.42
1:D:168:PHE:CE1	1:D:186:CYS:HB3	2.55	0.42
1:B:240:GLN:HA	1:B:246:VAL:O	2.19	0.42
1:C:188:GLN:HB3	1:C:267:VAL:HG13	2.01	0.42
1:C:218:GLU:CD	1:C:218:GLU:H	2.23	0.42
1:B:147:HIS:HB3	1:B:191:HIS:O	2.18	0.42
1:A:176:TRP:HB2	1:A:177:PRO:HD2	2.00	0.42
1:D:188:GLN:HB3	1:D:267:VAL:HG13	2.00	0.42
1:C:40:ARG:NH2	1:C:53:ARG:NH2	2.68	0.42
1:D:162:PHE:HD2	1:D:168:PHE:CE2	2.38	0.42
1:D:142:ILE:HG22	1:D:187:ASN:HD22	1.85	0.42
1:C:168:PHE:HD1	1:C:186:CYS:CA	2.30	0.41
1:D:217:LYS:CE	1:D:247:TYR:CE1	3.01	0.41
1:C:67:TRP:NE1	1:C:115:HIS:ND1	2.52	0.41
1:C:69:VAL:CG2	1:C:74:LEU:HD13	2.49	0.41
1:C:8:TYR:OH	1:C:116:GLU:OE1	2.33	0.41
1:D:64:ALA:HB1	1:D:116:GLU:CD	2.40	0.41
1:C:6:LEU:HG	1:C:145:LEU:CD2	2.51	0.41
1:A:232:TYR:CD2	3:A:302:P6G:H51	2.55	0.41
1:C:21:MET:CE	1:C:25:TYR:CE2	3.03	0.41
1:D:172:ASP:OD2	1:D:190:HIS:NE2	2.46	0.41
1:C:174:VAL:HG23	1:C:183:PHE:CE2	2.55	0.41
1:C:138:GLU:OE2	1:C:215:LYS:NZ	2.47	0.41
1:A:176:TRP:NE1	1:A:178:GLU:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:SER:HA	1:D:274:TRP:HE1	1.86	0.41
1:A:67:TRP:HH2	1:A:193:VAL:CG2	2.33	0.41
1:A:176:TRP:NE1	1:A:178:GLU:OE2	2.47	0.41
1:D:19:GLU:CD	1:D:35:ARG:HH22	2.24	0.41
1:C:34:GLU:OE2	1:C:44:ARG:NH1	2.42	0.41
1:C:46:ASP:CA	1:C:129:LEU:HD23	2.51	0.41
1:A:246:VAL:CG1	1:A:248:SER:HB3	2.52	0.41
1:D:142:ILE:HG22	1:D:187:ASN:ND2	2.36	0.40
1:D:150:VAL:HG22	1:D:195:LEU:HD23	2.03	0.40
1:D:128:VAL:CG2	1:D:129:LEU:N	2.84	0.40
1:D:155:ARG:NE	1:D:182:PHE:CD2	2.89	0.40
1:C:10:ILE:HD11	1:C:99:ARG:HD2	2.02	0.40
1:C:21:MET:CE	1:C:25:TYR:HE2	2.34	0.40
1:C:43:VAL:HB	1:C:52:ILE:HB	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	287/294 (98%)	283 (99%)	4 (1%)	0	100	100
1	B	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	C	287/294 (98%)	282 (98%)	5 (2%)	0	100	100
1	D	287/294 (98%)	282 (98%)	5 (2%)	0	100	100
All	All	1148/1176 (98%)	1128 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	231/235 (98%)	228 (99%)	3 (1%)	76	82
1	B	231/235 (98%)	229 (99%)	2 (1%)	84	89
1	C	231/235 (98%)	227 (98%)	4 (2%)	68	74
1	D	231/235 (98%)	228 (99%)	3 (1%)	76	82
All	All	924/940 (98%)	912 (99%)	12 (1%)	76	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	245	LYS
1	A	290	GLN
1	B	3	VAL
1	B	245	LYS
1	C	111	ASP
1	C	125	THR
1	C	218	GLU
1	C	290	GLN
1	D	18	LEU
1	D	222	ARG
1	D	233	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	ASN
1	D	275	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	P6G	A	302	-	18,18,18	0.50	0	17,17,17	0.35	0
4	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.08	0
3	P6G	B	302	-	18,18,18	0.46	0	17,17,17	0.56	0
4	SO4	B	303	-	4,4,4	0.19	0	6,6,6	0.14	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
3	P6G	A	302	-	-	0/16/16/16	0/0/0/0
4	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	P6G	B	302	-	-	0/16/16/16	0/0/0/0
4	SO4	B	303	-	-	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.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	P6G	2	0
3	B	302	P6G	9	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	289/294 (98%)	0.82	39 (13%)	4 6	11, 23, 37, 46	289 (100%)
1	B	289/294 (98%)	0.84	49 (16%)	2 3	11, 23, 37, 45	289 (100%)
1	C	289/294 (98%)	5.82	208 (71%)	0 0	11, 23, 37, 44	289 (100%)
1	D	289/294 (98%)	5.69	233 (80%)	0 0	11, 23, 36, 44	289 (100%)
All	All	1156/1176 (98%)	3.29	529 (45%)	0 0	11, 23, 37, 46	1156 (100%)

All (529) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	TYR	29.5
1	C	227	VAL	24.3
1	C	28	ILE	22.9
1	D	123	PHE	20.8
1	C	152	VAL	20.8
1	D	62	LEU	19.5
1	C	91	ALA	18.8
1	C	71	PRO	18.5
1	C	230	LEU	18.4
1	C	258	ALA	17.9
1	C	95	LEU	17.1
1	D	60	ASN	17.1
1	C	226	ALA	17.0
1	C	229	ARG	16.9
1	D	163	THR	16.7
1	C	43	VAL	16.6
1	D	276	VAL	16.6
1	C	259	VAL	16.5
1	C	274	TRP	16.5
1	D	122	SER	16.2
1	C	251	MET	15.9

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Mol	Chain	Res	Type	RSRZ
1	C	156	ALA	15.7
1	C	252	MET	15.6
1	C	50	PHE	15.2
1	C	257	PHE	15.2
1	C	93	ALA	15.0
1	C	139	ALA	14.7
1	C	268	ILE	14.5
1	D	182	PHE	14.5
1	B	200	LEU	14.4
1	D	145	LEU	14.3
1	D	170	LEU	14.3
1	C	202	LEU	14.2
1	D	11	PHE	13.9
1	D	267	VAL	13.8
1	C	153	ALA	13.7
1	D	200	LEU	13.7
1	C	210	LEU	13.3
1	D	255	ALA	13.3
1	D	10	ILE	13.2
1	C	100	ALA	13.1
1	D	257	PHE	13.1
1	C	231	GLY	13.0
1	D	63	ALA	13.0
1	D	9	LEU	12.8
1	D	275	HIS	12.8
1	C	233	ASP	12.7
1	C	70	ASP	12.7
1	C	154	ASP	12.6
1	C	184	LEU	12.6
1	D	212	LEU	12.6
1	D	42	LEU	12.5
1	C	32	VAL	12.4
1	D	168	PHE	12.4
1	D	184	LEU	12.3
1	D	278	PHE	12.2
1	C	151	ILE	12.2
1	D	29	ILE	12.0
1	C	170	LEU	12.0
1	D	261	LEU	11.8
1	C	267	VAL	11.8
1	D	33	VAL	11.8
1	D	54	LEU	11.6

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Mol	Chain	Res	Type	RSRZ
1	C	92	ASP	11.5
1	C	203	LYS	11.4
1	C	147	HIS	11.4
1	D	48	ARG	11.3
1	C	155	ARG	11.3
1	D	193	VAL	11.3
1	C	81	VAL	11.2
1	D	64	ALA	11.2
1	C	99	ARG	11.2
1	D	274	TRP	11.1
1	C	235	LEU	11.0
1	C	72	SER	11.0
1	D	77	ILE	11.0
1	C	234	VAL	10.9
1	B	85	CYS	10.9
1	D	6	LEU	10.8
1	D	61	ARG	10.7
1	C	197	ALA	10.7
1	C	42	LEU	10.7
1	C	27	ASP	10.6
1	D	50	PHE	10.6
1	D	22	VAL	10.6
1	D	30	GLY	10.6
1	D	91	ALA	10.4
1	C	118	TYR	10.4
1	C	169	GLY	10.4
1	D	49	PRO	10.3
1	A	200	LEU	10.2
1	D	231	GLY	10.2
1	C	269	GLY	10.2
1	C	266	GLN	10.2
1	D	186	CYS	10.1
1	D	254	PRO	10.1
1	D	273	SER	10.0
1	D	166	LEU	9.9
1	C	196	SER	9.9
1	D	121	SER	9.9
1	C	250	TYR	9.8
1	C	44	ARG	9.8
1	C	275	HIS	9.7
1	D	169	GLY	9.7
1	C	52	ILE	9.6

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Mol	Chain	Res	Type	RSRZ
1	C	193	VAL	9.6
1	C	277	GLY	9.6
1	C	186	CYS	9.6
1	D	39	GLY	9.5
1	C	3	VAL	9.4
1	D	12	GLU	9.4
1	D	268	ILE	9.4
1	D	100	ALA	9.4
1	C	189	ARG	9.3
1	C	185	HIS	9.3
1	C	209	HIS	9.3
1	D	66	GLY	9.2
1	D	181	ILE	9.2
1	C	195	LEU	9.2
1	C	246	VAL	9.2
1	D	7	GLY	9.2
1	D	178	GLU	9.1
1	C	8	TYR	9.1
1	C	171	SER	9.1
1	D	271	LEU	9.1
1	C	214	ALA	9.1
1	D	38	GLY	9.1
1	C	49	PRO	9.0
1	D	189	ARG	8.9
1	D	41	ALA	8.9
1	D	247	TYR	8.9
1	C	244	ASP	8.8
1	D	246	VAL	8.8
1	D	28	ILE	8.8
1	C	7	GLY	8.8
1	D	8	TYR	8.7
1	D	144	GLY	8.7
1	C	278	PHE	8.7
1	C	273	SER	8.7
1	C	253	ALA	8.6
1	C	228	LYS	8.6
1	C	183	PHE	8.6
1	C	284	ILE	8.5
1	D	256	GLY	8.5
1	D	78	ALA	8.5
1	D	101	ALA	8.5
1	C	13	CYS	8.5

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Mol	Chain	Res	Type	RSRZ
1	C	279	TYR	8.4
1	D	269	GLY	8.4
1	C	271	LEU	8.4
1	D	192	THR	8.4
1	D	95	LEU	8.4
1	D	265	GLY	8.3
1	D	277	GLY	8.3
1	D	221	ASP	8.3
1	D	187	ASN	8.2
1	C	33	VAL	8.2
1	C	96	ALA	8.2
1	C	98	ASP	8.2
1	D	47	GLY	8.2
1	C	276	VAL	8.2
1	D	162	PHE	8.1
1	C	31	ALA	8.1
1	D	210	LEU	8.1
1	C	285	TRP	8.1
1	D	148	LEU	8.1
1	A	177	PRO	8.0
1	D	23	VAL	8.0
1	D	117	LEU	8.0
1	C	241	HIS	8.0
1	C	34	GLU	8.0
1	D	102	ALA	7.9
1	D	93	ALA	7.9
1	C	201	GLY	7.8
1	D	97	ALA	7.8
1	D	180	ASP	7.8
1	C	213	GLU	7.8
1	D	173	ARG	7.7
1	D	234	VAL	7.7
1	C	101	ALA	7.7
1	D	146	GLY	7.6
1	D	20	GLN	7.6
1	D	171	SER	7.6
1	C	187	ASN	7.6
1	D	52	ILE	7.6
1	D	3	VAL	7.6
1	C	9	LEU	7.4
1	C	62	LEU	7.4
1	C	104	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
1	C	191	HIS	7.3
1	C	190	HIS	7.2
1	A	176	TRP	7.2
1	D	149	VAL	7.2
1	B	177	PRO	7.1
1	D	211	MET	7.0
1	D	183	PHE	7.0
1	D	238	ILE	7.0
1	D	167	GLY	7.0
1	B	178	GLU	6.9
1	D	104	VAL	6.9
1	C	5	GLN	6.9
1	C	242	SER	6.9
1	C	207	VAL	6.8
1	C	260	GLU	6.8
1	C	180	ASP	6.8
1	C	150	VAL	6.8
1	D	208	HIS	6.8
1	C	24	VAL	6.8
1	D	31	ALA	6.8
1	D	201	GLY	6.8
1	C	199	ALA	6.7
1	D	188	GLN	6.7
1	D	119	VAL	6.7
1	C	2	SER	6.7
1	D	279	TYR	6.6
1	C	68	ASN	6.6
1	D	213	GLU	6.6
1	D	222	ARG	6.5
1	D	69	VAL	6.4
1	C	4	LYS	6.4
1	C	94	GLU	6.4
1	D	239	GLY	6.4
1	D	34	GLU	6.4
1	D	2	SER	6.4
1	D	43	VAL	6.4
1	D	270	ASP	6.4
1	C	239	GLY	6.4
1	D	51	ARG	6.4
1	D	24	VAL	6.4
1	D	53	ARG	6.3
1	C	146	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	204	PRO	6.3
1	C	182	PHE	6.3
1	D	179	ALA	6.3
1	C	38	GLY	6.3
1	C	188	GLN	6.3
1	D	103	GLN	6.3
1	C	208	HIS	6.3
1	C	237	THR	6.3
1	C	53	ARG	6.2
1	C	74	LEU	6.1
1	C	135	CYS	6.1
1	D	67	TRP	6.1
1	D	185	HIS	6.1
1	D	96	ALA	6.0
1	D	258	ALA	6.0
1	C	26	GLN	6.0
1	C	200	LEU	6.0
1	D	74	LEU	5.9
1	D	25	TYR	5.9
1	A	179	ALA	5.9
1	B	199	ALA	5.9
1	D	76	ALA	5.9
1	D	99	ARG	5.9
1	D	5	GLN	5.9
1	D	266	GLN	5.9
1	D	40	ARG	5.9
1	B	176	TRP	5.8
1	A	178	GLU	5.8
1	C	194	ALA	5.8
1	D	55	ASP	5.8
1	D	27	ASP	5.8
1	A	128	VAL	5.7
1	C	149	VAL	5.7
1	D	147	HIS	5.6
1	D	56	PRO	5.6
1	D	209	HIS	5.6
1	D	35	ARG	5.6
1	C	36	ASP	5.6
1	D	259	VAL	5.6
1	D	245	LYS	5.6
1	B	179	ALA	5.6
1	D	191	HIS	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	120	GLU	5.5
1	C	145	LEU	5.5
1	D	118	TYR	5.5
1	D	92	ASP	5.5
1	B	231	GLY	5.4
1	D	17	VAL	5.4
1	C	166	LEU	5.4
1	C	236	MET	5.4
1	C	270	ASP	5.3
1	C	243	ASN	5.3
1	D	194	ALA	5.3
1	D	172	ASP	5.3
1	C	168	PHE	5.3
1	D	36	ASP	5.2
1	D	220	VAL	5.2
1	D	280	ASP	5.2
1	A	231	GLY	5.2
1	D	272	GLU	5.1
1	C	6	LEU	5.1
1	C	206	MET	5.1
1	C	172	ASP	5.1
1	D	284	ILE	5.1
1	D	21	MET	5.1
1	D	190	HIS	5.1
1	D	174	VAL	5.0
1	C	177	PRO	5.0
1	C	111	ASP	5.0
1	D	94	GLU	5.0
1	A	199	ALA	4.9
1	D	175	THR	4.9
1	B	201	GLY	4.9
1	C	97	ALA	4.9
1	A	127	PRO	4.8
1	D	75	ALA	4.8
1	D	65	ILE	4.8
1	C	73	ASP	4.8
1	A	289	LEU	4.8
1	C	35	ARG	4.8
1	A	201	GLY	4.7
1	B	290	GLN	4.7
1	D	98	ASP	4.7
1	C	211	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	85	CYS	4.7
1	C	37	GLU	4.7
1	C	192	THR	4.7
1	C	105	ARG	4.7
1	D	230	LEU	4.6
1	C	90	THR	4.6
1	C	69	VAL	4.6
1	D	4	LYS	4.6
1	D	176	TRP	4.6
1	C	21	MET	4.6
1	C	181	ILE	4.6
1	D	88	VAL	4.6
1	A	154	ASP	4.5
1	D	68	ASN	4.5
1	D	285	TRP	4.5
1	C	216	SER	4.5
1	D	283	SER	4.5
1	D	232	TYR	4.5
1	D	253	ALA	4.4
1	C	256	GLY	4.4
1	D	131	SER	4.4
1	D	159	GLN	4.3
1	A	233	ASP	4.3
1	D	109	ASP	4.2
1	C	174	VAL	4.2
1	C	198	PRO	4.2
1	D	142	ILE	4.2
1	C	287	HIS	4.1
1	C	290	GLN	4.1
1	D	26	GLN	4.1
1	D	262	GLY	4.1
1	D	263	PHE	4.1
1	D	223	ALA	4.1
1	C	141	GLY	4.0
1	D	80	GLN	4.0
1	C	66	GLY	4.0
1	C	10	ILE	3.9
1	D	226	ALA	3.9
1	D	252	MET	3.9
1	D	281	ALA	3.9
1	C	283	SER	3.9
1	A	175	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	176	TRP	3.8
1	D	150	VAL	3.8
1	C	125	THR	3.8
1	C	175	THR	3.8
1	C	245	LYS	3.8
1	D	249	PHE	3.8
1	B	288	GLU	3.8
1	B	164	ASP	3.7
1	A	232	TYR	3.7
1	B	202	LEU	3.7
1	C	179	ALA	3.7
1	B	275	HIS	3.7
1	A	290	GLN	3.7
1	C	29	ILE	3.7
1	D	228	LYS	3.7
1	D	143	PHE	3.7
1	D	37	GLU	3.6
1	A	285	TRP	3.6
1	B	124	PRO	3.6
1	D	45	LEU	3.6
1	D	248	SER	3.6
1	C	117	LEU	3.6
1	D	116	GLU	3.5
1	B	280	ASP	3.5
1	D	165	VAL	3.5
1	D	236	MET	3.5
1	A	203	LYS	3.5
1	A	125	THR	3.5
1	C	102	ALA	3.5
1	D	227	VAL	3.5
1	A	288	GLU	3.5
1	D	71	PRO	3.4
1	D	32	VAL	3.4
1	D	134	VAL	3.4
1	D	128	VAL	3.4
1	B	180	ASP	3.4
1	B	272	GLU	3.4
1	C	289	LEU	3.4
1	D	157	LYS	3.3
1	D	135	CYS	3.3
1	C	48	ARG	3.3
1	D	90	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	3.3
1	D	13	CYS	3.3
1	D	160	SER	3.3
1	D	127	PRO	3.3
1	D	289	LEU	3.3
1	D	233	ASP	3.3
1	D	70	ASP	3.3
1	D	225	ALA	3.2
1	D	202	LEU	3.2
1	D	235	LEU	3.2
1	D	264	GLY	3.2
1	B	154	ASP	3.2
1	C	67	TRP	3.2
1	D	229	ARG	3.2
1	D	199	ALA	3.2
1	D	237	THR	3.2
1	A	234	VAL	3.2
1	C	165	VAL	3.2
1	C	240	GLN	3.1
1	C	54	LEU	3.1
1	D	240	GLN	3.1
1	C	225	ALA	3.1
1	B	130	GLU	3.1
1	B	128	VAL	3.0
1	C	82	GLU	3.0
1	B	125	THR	3.0
1	A	157	LYS	3.0
1	D	250	TYR	3.0
1	C	51	ARG	3.0
1	C	248	SER	3.0
1	D	241	HIS	3.0
1	C	247	TYR	2.9
1	B	94	GLU	2.9
1	B	139	ALA	2.9
1	D	124	PRO	2.9
1	B	216	SER	2.9
1	B	218	GLU	2.9
1	C	57	GLY	2.9
1	C	144	GLY	2.9
1	A	139	ALA	2.9
1	C	65	ILE	2.8
1	C	282	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	203	LYS	2.8
1	C	40	ARG	2.8
1	C	224	PHE	2.8
1	A	270	ASP	2.8
1	B	79	GLU	2.8
1	D	196	SER	2.8
1	C	286	GLY	2.8
1	D	108	ALA	2.8
1	B	175	THR	2.8
1	C	136	GLY	2.7
1	C	262	GLY	2.7
1	D	44	ARG	2.7
1	B	38	GLY	2.7
1	B	57	GLY	2.7
1	B	232	TYR	2.7
1	B	153	ALA	2.7
1	A	280	ASP	2.7
1	D	18	LEU	2.7
1	C	173	ARG	2.7
1	C	86	TYR	2.7
1	B	278	PHE	2.7
1	D	106	GLN	2.6
1	B	289	LEU	2.6
1	A	153	ALA	2.6
1	A	37	GLU	2.6
1	D	72	SER	2.6
1	C	137	GLU	2.6
1	D	105	ARG	2.6
1	A	124	PRO	2.5
1	C	261	LEU	2.5
1	C	238	ILE	2.5
1	D	242	SER	2.5
1	D	260	GLU	2.5
1	A	229	ARG	2.5
1	B	229	ARG	2.5
1	D	224	PHE	2.5
1	D	251	MET	2.5
1	C	272	GLU	2.5
1	D	243	ASN	2.5
1	A	180	ASP	2.5
1	A	216	SER	2.5
1	D	288	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	233	ASP	2.5
1	D	161	PHE	2.5
1	C	30	GLY	2.5
1	B	80	GLN	2.5
1	D	57	GLY	2.4
1	B	76	ALA	2.4
1	C	281	ALA	2.4
1	B	97	ALA	2.4
1	A	198	PRO	2.4
1	D	217	LYS	2.4
1	B	84	ALA	2.3
1	C	249	PHE	2.3
1	C	263	PHE	2.3
1	C	55	ASP	2.3
1	C	219	GLN	2.3
1	B	127	PRO	2.3
1	B	198	PRO	2.3
1	C	76	ALA	2.3
1	C	280	ASP	2.3
1	C	15	ALA	2.3
1	B	111	ASP	2.3
1	C	220	VAL	2.3
1	B	123	PHE	2.2
1	C	140	ASN	2.2
1	D	73	ASP	2.2
1	C	113	PHE	2.2
1	D	152	VAL	2.2
1	A	284	ILE	2.2
1	D	244	ASP	2.2
1	B	234	VAL	2.2
1	D	151	ILE	2.2
1	C	18	LEU	2.2
1	D	133	PHE	2.2
1	A	228	LYS	2.2
1	D	177	PRO	2.2
1	A	268	ILE	2.1
1	C	60	ASN	2.1
1	A	94	GLU	2.1
1	C	39	GLY	2.1
1	B	285	TRP	2.1
1	D	216	SER	2.0
1	B	207	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	12	GLU	2.0
1	A	123	PHE	2.0
1	B	237	THR	2.0
1	C	77	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
4	SO4	B	303	5/5	0.96	0.24	0.21	46,46,47,48	5
3	P6G	A	302	19/19	0.81	0.21	0.11	42,46,52,53	19
4	SO4	A	303	5/5	0.96	0.18	0.06	48,48,50,50	5
3	P6G	B	302	19/19	0.85	0.20	-0.54	36,39,46,48	19
2	FE2	D	300	1/1	0.96	0.33	-0.82	20,20,20,20	1
2	FE2	C	300	1/1	0.96	0.32	-1.88	20,20,20,20	1
2	FE2	B	301	1/1	1.00	0.05	-2.25	20,20,20,20	1
2	FE2	A	301	1/1	0.99	0.05	-3.61	21,21,21,21	1

6.5 Other polymers (i)

There are no such residues in this entry.