



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MMB
Title : Dissimilatory sulfite reductase in complex with the endproduct sulfide
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

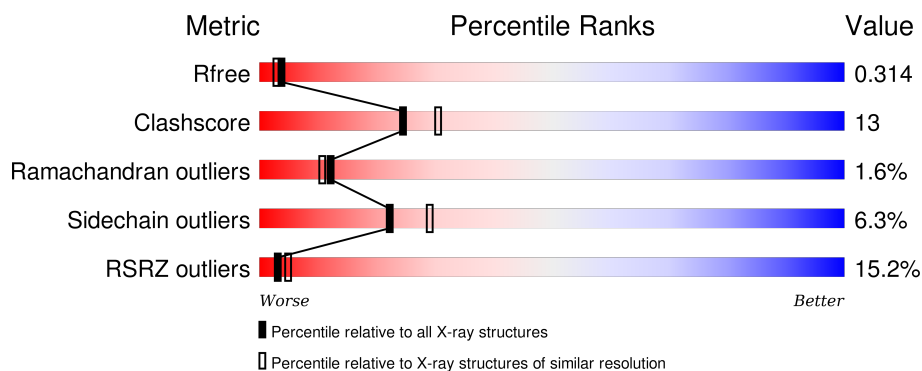
1 Overall quality at a glance

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 $\leq 5\%$. 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	418	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	D	418	<div> <div>28%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
2	B	366	<div> <div>%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
2	E	366	<div> <div>28%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>

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	SRM	A	580	-	-	X	-
4	SF4	B	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12893 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.

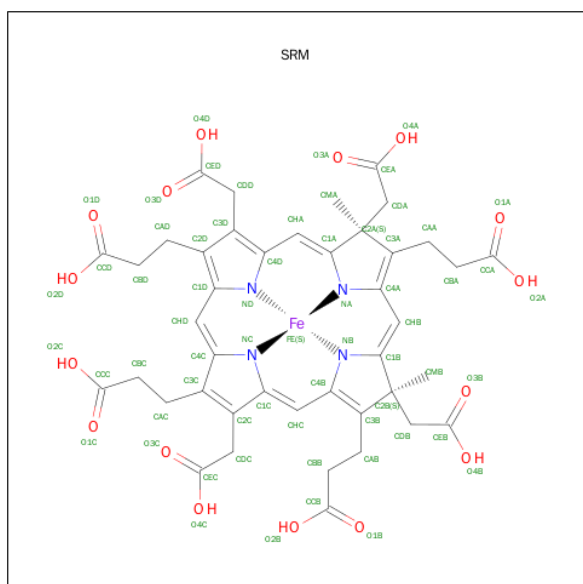
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			
1	D	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			

- Molecule 2 is a protein called Sulfite reductase, dissimilatory-type subunit beta.

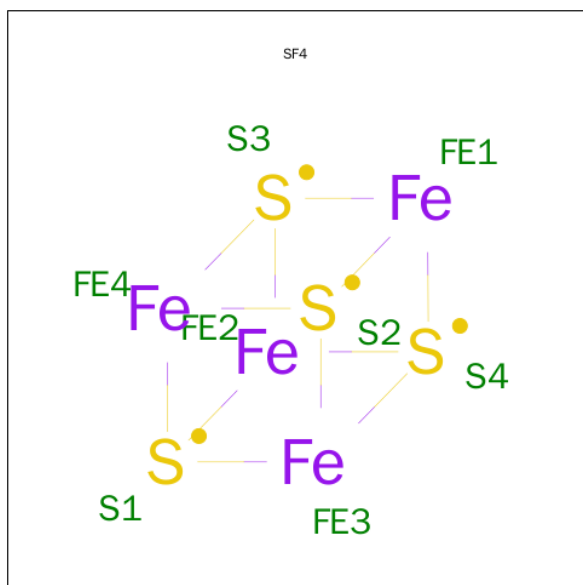
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



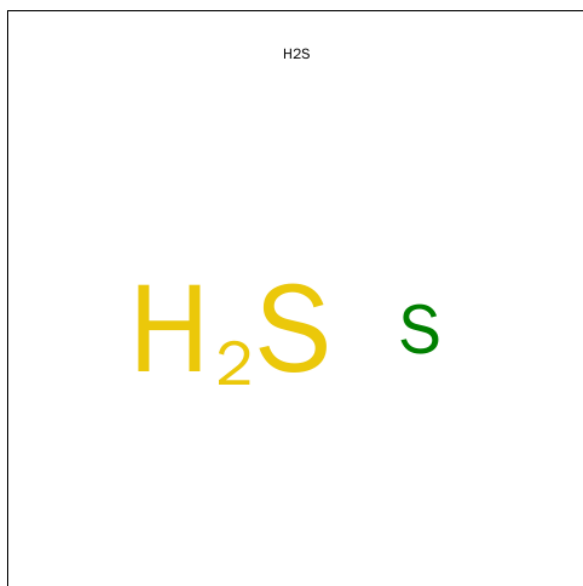
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S		
			8	4	4	0	0
4	A	1	Total	Fe	S		
			8	4	4	0	0
4	B	1	Total	Fe	S		
			8	4	4	0	0
4	B	1	Total	Fe	S		
			8	4	4	0	0
4	D	1	Total	Fe	S		
			8	4	4	0	0
4	D	1	Total	Fe	S		
			8	4	4	0	0
4	E	1	Total	Fe	S		
			8	4	4	0	0
4	E	1	Total	Fe	S		
			8	4	4	0	0

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H₂S) (formula: H₂S).



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

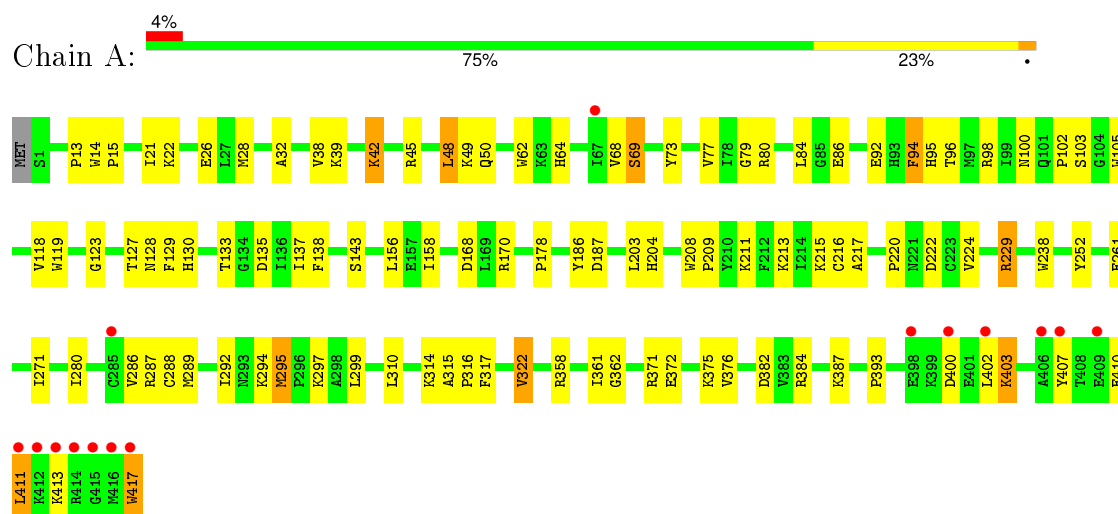
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0
6	B	36	Total O 36 36	0	0
6	D	33	Total O 33 33	0	0
6	E	13	Total O 13 13	0	0

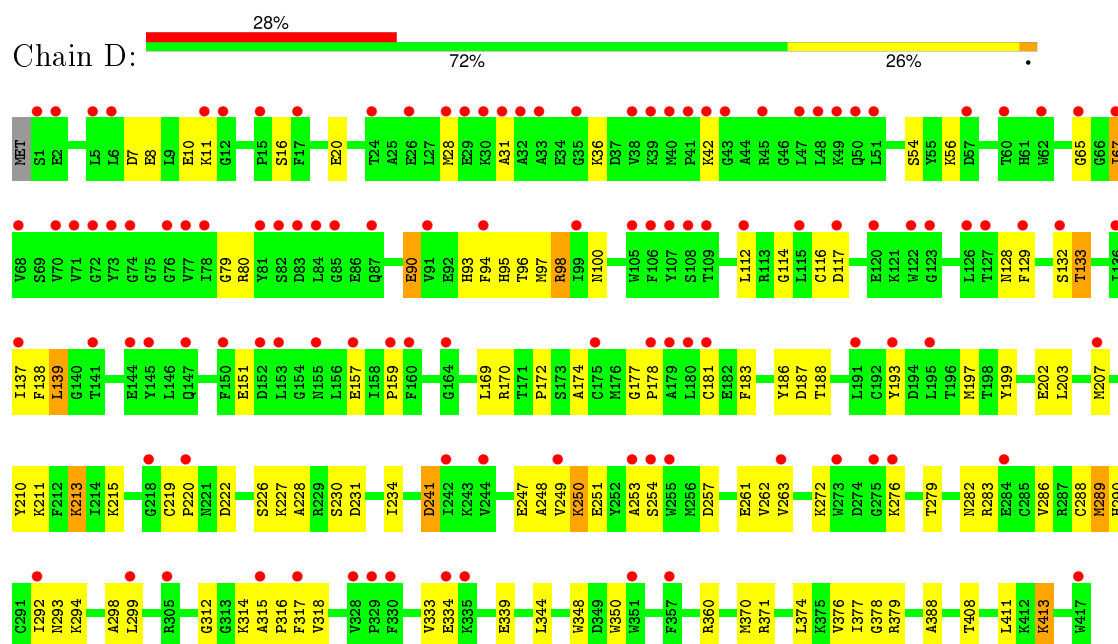
3 Residue-property plots

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.

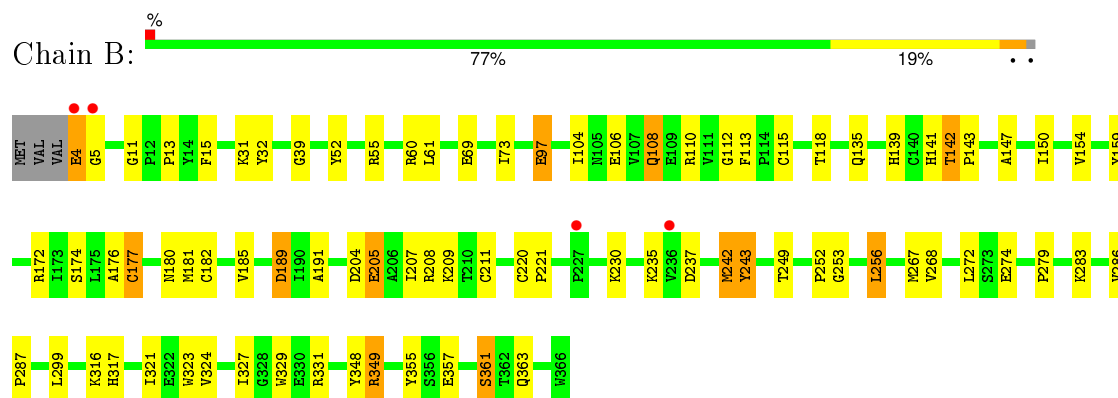
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



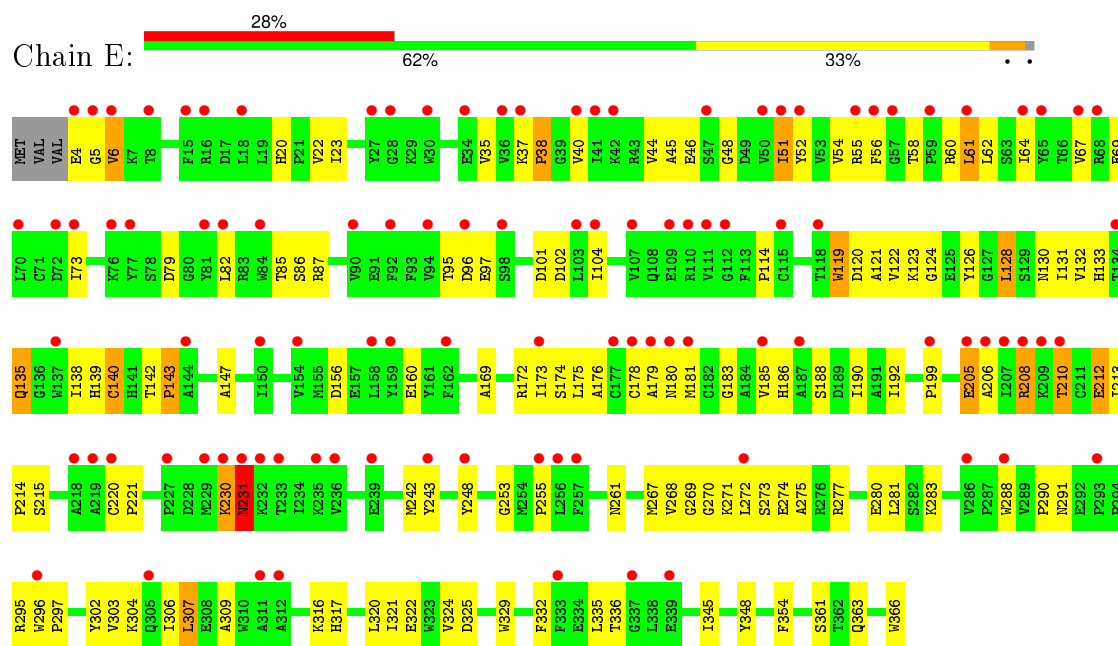
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 68.50Å 146.50Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 93.0 (19.96-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.255 , 0.302 0.269 , 0.314	Depositor DCC
R_{free} test set	3960 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 4.2	EDS
Estimated twinning fraction	0.159 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 79202 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12893	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, H2S, SRM

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	0.70	0/3417	0.77	2/4610 (0.0%)
1	D	0.49	0/3417	0.62	0/4610
2	B	0.74	1/2984 (0.0%)	0.80	0/4058
2	E	0.48	0/2984	0.67	1/4058 (0.0%)
All	All	0.61	1/12802 (0.0%)	0.72	3/17336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	177	CYS	CB-SG	-7.84	1.69	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	61	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	411	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	84	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3330	0	3276	82	0
1	D	3330	0	3276	89	0
2	B	2901	0	2838	70	0
2	E	2901	0	2839	106	0
3	A	63	0	34	24	0
3	B	63	0	34	7	0
3	D	63	0	34	13	0
3	E	63	0	34	13	0
4	A	16	0	0	0	0
4	B	16	0	0	2	0
4	D	16	0	0	1	0
4	E	16	0	0	1	0
5	A	1	0	0	0	0
6	A	32	0	0	1	0
6	B	36	0	0	1	0
6	D	33	0	0	6	0
6	E	13	0	0	4	0
All	All	12893	0	12365	322	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 13.

All (322) 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)
4:D:575:SF4:S4	6:D:439:HOH:O	1.93	1.21
1:D:315:ALA:HB1	1:D:316:PRO:HD2	1.26	1.14
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.29	1.07
1:D:413:LYS:NZ	6:D:430:HOH:O	1.96	0.97
1:D:211:LYS:HD3	1:D:213:LYS:HE3	1.45	0.96
2:E:121:ALA:HB2	3:E:570:SRM:O3D	1.65	0.95
1:A:215:LYS:HE2	1:A:229:ARG:HD3	1.48	0.93
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.99	0.93
1:A:80:ARG:NH2	3:A:580:SRM:O2A	2.02	0.92
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.37	0.88
2:E:140:CYS:HG	4:E:585:SF4:FE2	0.79	0.87
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.58	0.84
2:B:274:GLU:OE1	2:B:363:GLN:NE2	2.10	0.84
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.60	0.84
1:D:183:PHE:HB2	6:D:439:HOH:O	1.79	0.82
1:D:170:ARG:HG3	1:D:213:LYS:HE2	1.62	0.81
3:E:570:SRM:O4D	3:E:570:SRM:HHA	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.10	0.80
1:A:314:LYS:HG2	1:A:322:VAL:HG23	1.64	0.80
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.64	0.79
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.63	0.79
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.23	0.78
2:B:349:ARG:HH11	2:B:349:ARG:HG3	1.48	0.78
1:D:211:LYS:CD	1:D:213:LYS:HE3	2.14	0.77
2:B:185:VAL:HG12	2:B:191:ALA:HB1	1.67	0.77
2:B:349:ARG:HA	2:E:354:PHE:HE2	1.50	0.76
1:A:413:LYS:HG2	1:A:413:LYS:O	1.85	0.75
3:D:580:SRM:HHB	3:D:580:SRM:HBA2	1.68	0.75
2:E:309:ALA:HB3	2:E:336:THR:HG22	1.68	0.75
1:D:219:CYS:SG	6:D:439:HOH:O	2.44	0.74
2:E:86:SER:OG	3:E:570:SRM:HAB1	1.87	0.74
1:D:317:PHE:HE2	2:E:180:ASN:HD22	1.34	0.74
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.71	0.73
2:E:126:TYR:CD1	2:E:169:ALA:HA	2.23	0.73
1:A:417:TRP:CD1	1:A:417:TRP:C	2.63	0.72
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.72	0.72
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.19	0.72
2:B:349:ARG:HA	2:E:354:PHE:CE2	2.25	0.71
2:E:128:LEU:HD21	2:E:173:ILE:HD12	1.74	0.70
1:D:248:ALA:HB3	1:D:298:ALA:HB2	1.72	0.69
1:A:322:VAL:HG12	2:B:355:TYR:CZ	2.27	0.69
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.14	0.69
1:A:403:LYS:HB3	2:E:261:ASN:OD1	1.93	0.68
1:D:215:LYS:HG3	1:D:230:SER:HB3	1.74	0.68
2:B:176:ALA:HB2	2:B:185:VAL:HG21	1.74	0.68
3:A:580:SRM:O1A	2:B:139:HIS:CD2	2.45	0.68
1:A:322:VAL:HG12	2:B:355:TYR:CE1	2.28	0.68
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.73	0.67
2:B:205:GLU:OE2	2:B:209:LYS:NZ	2.28	0.67
1:D:374:LEU:HB3	1:D:379:ARG:O	1.95	0.66
1:A:127:THR:O	2:B:61:LEU:HD12	1.95	0.66
2:E:199:PRO:HA	6:E:377:HOH:O	1.95	0.66
3:E:570:SRM:HDA1	6:E:376:HOH:O	1.94	0.66
1:D:16:SER:O	1:D:20:GLU:HG2	1.96	0.66
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.27	0.65
3:D:580:SRM:CDD	3:D:580:SRM:HBD2	2.26	0.65
1:D:211:LYS:NZ	3:D:580:SRM:HDD2	2.12	0.64
1:D:133:THR:OG1	3:D:580:SRM:HAB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:O	1:A:69:SER:HB3	1.97	0.64
2:E:55:ARG:NH2	3:E:570:SRM:HBA2	2.11	0.64
1:A:62:TRP:HB3	1:A:80:ARG:HD2	1.80	0.63
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.29	0.63
1:A:288:CYS:O	1:A:289:MET:HB2	1.98	0.62
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.81	0.62
1:D:65:GLY:H	1:D:80:ARG:NH1	1.98	0.62
1:A:186:TYR:OH	1:A:216:CYS:HB3	2.00	0.62
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.81	0.62
1:D:249:VAL:HG23	1:D:298:ALA:HB1	1.82	0.62
2:E:206:ALA:O	2:E:210:THR:OG1	2.19	0.61
2:E:212:GLU:HB2	6:E:374:HOH:O	2.01	0.61
1:A:271:ILE:HD12	1:A:280:ILE:HG12	1.83	0.61
1:A:211:LYS:NZ	3:A:580:SRM:HAD1	2.15	0.60
2:B:189:ASP:O	2:B:268:VAL:HA	2.01	0.60
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.34	0.60
1:D:286:VAL:HB	2:E:363:GLN:HG3	1.84	0.59
1:A:94:PHE:O	2:B:139:HIS:HE1	1.86	0.59
1:A:68:VAL:HG13	1:A:77:VAL:HG12	1.83	0.59
2:E:291:ASN:HA	2:E:296:TRP:HE1	1.68	0.59
1:D:317:PHE:HE2	2:E:180:ASN:ND2	1.99	0.58
2:B:331:ARG:NH2	2:E:366:TRP:O	2.36	0.58
1:A:96:THR:HG23	2:B:139:HIS:NE2	2.18	0.58
3:A:580:SRM:HMB1	3:A:580:SRM:CBB	2.34	0.58
2:E:51:ILE:HD12	2:E:95:THR:HG22	1.84	0.58
2:B:142:THR:N	2:B:143:PRO:CD	2.66	0.58
1:D:315:ALA:CB	1:D:316:PRO:HD2	2.13	0.58
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	1.86	0.58
1:D:371:ARG:NH1	6:D:418:HOH:O	2.26	0.58
2:B:55:ARG:O	2:B:115:CYS:HA	2.04	0.58
3:D:580:SRM:HBD2	3:D:580:SRM:HDD1	1.87	0.57
3:D:580:SRM:O4D	3:D:580:SRM:HHA	2.04	0.57
1:D:292:ILE:HG23	1:D:299:LEU:O	2.05	0.57
2:B:349:ARG:NH1	2:B:349:ARG:HG3	2.17	0.57
1:A:292:ILE:HG23	1:A:299:LEU:O	2.04	0.56
2:E:175:LEU:HA	2:E:192:ILE:O	2.05	0.56
2:B:331:ARG:NH1	1:D:283:ARG:O	2.38	0.56
2:B:204:ASP:O	2:B:208:ARG:HG3	2.06	0.56
1:A:215:LYS:HE2	1:A:229:ARG:CD	2.30	0.56
1:A:64:HIS:HE1	2:B:249:THR:O	1.88	0.56
1:D:98:ARG:CZ	3:D:580:SRM:HMB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:HIS:HB2	2:E:147:ALA:HB1	1.88	0.56
2:E:304:LYS:C	2:E:306:ILE:H	2.08	0.56
1:A:98:ARG:HH21	3:A:580:SRM:HMB3	1.69	0.55
2:E:119:TRP:HE1	3:E:570:SRM:HDD2	1.70	0.55
1:D:183:PHE:HE2	1:D:293:ASN:OD1	1.90	0.55
1:A:45:ARG:O	1:A:49:LYS:HG3	2.06	0.55
1:D:183:PHE:CB	6:D:439:HOH:O	2.46	0.55
1:D:228:ALA:HB2	2:E:272:LEU:CD2	2.36	0.55
2:B:348:TYR:O	2:E:354:PHE:HD2	1.90	0.55
1:A:252:TYR:CD2	1:A:295:MET:HG3	2.42	0.55
1:A:286:VAL:CG2	2:B:363:GLN:HG2	2.36	0.54
2:B:52:TYR:CE1	2:B:97:GLU:HB3	2.42	0.54
1:D:181:CYS:SG	1:D:183:PHE:HB2	2.48	0.54
1:D:248:ALA:CB	1:D:298:ALA:HB2	2.36	0.54
2:E:316:LYS:O	2:E:317:HIS:HB2	2.07	0.54
3:B:570:SRM:CBA	3:B:570:SRM:HMA3	2.37	0.54
2:B:207:ILE:HG13	2:B:253:GLY:HA3	1.89	0.54
1:D:65:GLY:HA3	1:D:79:GLY:O	2.07	0.54
2:B:349:ARG:CA	2:E:354:PHE:HE2	2.19	0.54
2:E:172:ARG:HH21	3:E:570:SRM:C2C	2.21	0.54
1:A:393:PRO:HG3	2:E:181:MET:HE3	1.88	0.54
3:A:580:SRM:HDA2	4:B:585:SF4:S1	2.49	0.53
1:D:316:PRO:HG3	2:E:179:ALA:O	2.09	0.53
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.48	0.53
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.43	0.53
1:D:317:PHE:CE2	2:E:180:ASN:ND2	2.76	0.52
2:B:104:ILE:O	2:B:108:GLN:HG2	2.09	0.52
3:D:580:SRM:HDD2	3:D:580:SRM:HBD2	1.90	0.52
1:D:257:ASP:O	1:D:261:GLU:HB2	2.08	0.52
1:A:211:LYS:HZ2	3:A:580:SRM:HAD1	1.75	0.52
1:D:211:LYS:HZ1	3:D:580:SRM:HDD2	1.75	0.52
1:A:238:TRP:CZ2	1:A:287:ARG:HG2	2.44	0.52
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.91	0.52
1:D:288:CYS:O	1:D:289:MET:HB2	2.10	0.52
1:A:94:PHE:O	2:B:139:HIS:CE1	2.63	0.52
1:D:94:PHE:O	2:E:139:HIS:NE2	2.40	0.52
1:A:314:LYS:HG2	1:A:322:VAL:CG2	2.37	0.52
2:B:279:PRO:HD2	2:B:361:SER:HB2	1.92	0.52
1:A:21:ILE:HG21	1:A:48:LEU:HB2	1.91	0.51
2:E:156:ASP:OD2	2:E:295:ARG:NH1	2.41	0.51
1:D:199:TYR:HB3	1:D:202:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:SRM:CHB	3:D:580:SRM:HBA2	2.39	0.51
2:B:272:LEU:HD12	3:B:570:SRM:HBC1	1.93	0.51
2:B:108:GLN:NE2	2:B:113:PHE:O	2.44	0.51
1:A:135:ASP:OD1	3:A:580:SRM:O1B	2.29	0.51
1:D:231:ASP:CG	1:D:360:ARG:HH21	2.14	0.51
2:E:304:LYS:C	2:E:306:ILE:N	2.64	0.51
1:D:241:ASP:OD2	1:D:282:ASN:ND2	2.44	0.51
2:B:150:ILE:O	2:B:154:VAL:HG23	2.10	0.51
1:D:312:GLY:O	1:D:314:LYS:HG2	2.11	0.50
2:E:20:HIS:CE1	2:E:22:VAL:HB	2.47	0.50
1:A:403:LYS:HB2	1:A:403:LYS:NZ	2.27	0.50
2:E:40:VAL:HG13	2:E:54:VAL:HG22	1.93	0.50
1:A:13:PRO:HB2	2:B:159:TYR:CD1	2.47	0.50
1:D:28:MET:SD	2:E:64:ILE:HD11	2.51	0.50
1:A:118:VAL:HG21	1:A:156:LEU:HD11	1.94	0.50
1:A:372:GLU:O	1:A:376:VAL:HG23	2.12	0.49
1:A:102:PRO:HG3	2:B:13:PRO:HG2	1.93	0.49
1:A:79:GLY:HA2	1:A:95:HIS:ND1	2.27	0.49
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.47	0.49
2:B:242:MET:C	2:B:243:TYR:CG	2.85	0.49
1:D:112:LEU:HD12	2:E:82:LEU:HD21	1.95	0.49
2:B:211:CYS:SG	2:B:252:PRO:HD2	2.53	0.49
1:D:8:GLU:HA	1:D:11:LYS:HZ2	1.78	0.49
1:A:417:TRP:HD1	1:A:417:TRP:O	1.95	0.49
1:A:203:LEU:HD23	1:A:203:LEU:C	2.33	0.49
2:E:212:GLU:HB3	2:E:215:SER:OG	2.13	0.49
1:A:213:LYS:NZ	3:A:580:SRM:O1C	2.45	0.49
1:A:314:LYS:CG	1:A:322:VAL:HG23	2.39	0.49
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.11	0.49
2:E:173:ILE:HA	2:E:190:ILE:O	2.12	0.49
1:A:127:THR:O	2:B:61:LEU:CD1	2.61	0.49
2:E:102:ASP:O	6:E:370:HOH:O	2.20	0.49
1:A:103:SER:HB2	2:B:15:PHE:HB3	1.95	0.49
1:A:220:PRO:HB3	2:B:274:GLU:HG3	1.95	0.48
1:A:417:TRP:HD1	1:A:417:TRP:C	2.13	0.48
2:E:132:VAL:HG22	2:E:174:SER:OG	2.13	0.48
2:E:69:GLU:O	2:E:73:ILE:HG13	2.13	0.48
2:E:205:GLU:HG3	2:E:208:ARG:NH1	2.27	0.48
2:E:296:TRP:N	2:E:297:PRO:HD3	2.28	0.48
1:A:68:VAL:O	1:A:69:SER:CB	2.61	0.48
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:O	2:E:348:TYR:OH	2.27	0.48
2:E:51:ILE:HG13	2:E:52:TYR:H	1.78	0.48
1:D:377:ILE:HG13	1:D:379:ARG:HG2	1.96	0.48
2:B:141:HIS:O	6:B:382:HOH:O	2.20	0.48
2:B:108:GLN:O	2:B:112:GLY:HA2	2.13	0.47
2:B:256:LEU:H	2:B:256:LEU:HD23	1.79	0.47
2:E:142:THR:N	2:E:143:PRO:HD3	2.29	0.47
2:E:291:ASN:HA	2:E:296:TRP:NE1	2.28	0.47
1:D:215:LYS:HB2	1:D:226:SER:CB	2.44	0.47
1:A:252:TYR:CE2	1:A:295:MET:HG3	2.49	0.47
2:E:281:LEU:O	2:E:283:LYS:NZ	2.44	0.47
1:D:314:LYS:NZ	1:D:315:ALA:O	2.47	0.47
1:D:202:GLU:N	1:D:202:GLU:OE1	2.48	0.47
3:A:580:SRM:NC	2:B:182:CYS:HA	2.29	0.47
2:E:363:GLN:HB2	2:E:363:GLN:HE21	1.59	0.47
2:E:277:ARG:NH1	2:E:325:ASP:OD2	2.39	0.47
1:A:22:LYS:O	1:A:26:GLU:HG3	2.14	0.46
1:A:315:ALA:HB1	1:A:316:PRO:CD	2.45	0.46
1:A:382:ASP:OD1	1:A:384:ARG:HD2	2.14	0.46
2:E:37:LYS:HB2	2:E:38:PRO:HD2	1.97	0.46
2:E:176:ALA:CB	2:E:181:MET:HA	2.45	0.46
2:E:316:LYS:HG2	2:E:317:HIS:CD2	2.51	0.46
1:D:129:PHE:HB2	2:E:62:LEU:HD12	1.96	0.46
3:A:580:SRM:C3D	2:B:180:ASN:HB3	2.46	0.46
2:B:176:ALA:HB1	2:B:181:MET:HA	1.98	0.46
1:D:151:GLU:HG3	2:E:6:VAL:HG13	1.97	0.46
2:E:35:VAL:HG21	2:E:120:ASP:HB3	1.98	0.46
1:D:213:LYS:O	1:D:230:SER:HB2	2.16	0.46
2:E:302:TYR:O	2:E:306:ILE:HG13	2.16	0.46
2:E:268:VAL:HG13	2:E:320:LEU:HD22	1.98	0.46
2:B:39:GLY:HA2	2:B:118:THR:HG23	1.98	0.46
1:A:13:PRO:HB2	2:B:159:TYR:CE1	2.50	0.45
2:E:130:ASN:OD1	2:E:131:ILE:N	2.48	0.45
2:E:280:GLU:HG2	2:E:321:ILE:HG12	1.98	0.45
2:E:320:LEU:O	2:E:324:VAL:HG23	2.16	0.45
2:B:316:LYS:HG2	2:B:317:HIS:CD2	2.51	0.45
3:E:570:SRM:O2A	3:E:570:SRM:HMA3	2.16	0.45
2:E:274:GLU:OE1	2:E:361:SER:OG	2.34	0.45
1:D:116:CYS:SG	2:E:67:VAL:HB	2.56	0.45
1:D:211:LYS:HZ2	3:D:580:SRM:HDD2	1.81	0.45
3:B:570:SRM:C1A	3:B:570:SRM:HBA1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.98	0.45
2:E:283:LYS:HD3	2:E:329:TRP:CZ2	2.51	0.45
1:D:317:PHE:HB2	3:D:580:SRM:O1D	2.16	0.45
1:A:158:ILE:HD11	6:A:427:HOH:O	2.15	0.45
1:A:286:VAL:HG23	2:B:363:GLN:HG2	1.98	0.45
2:E:270:GLY:HA2	2:E:280:GLU:O	2.17	0.45
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.52	0.45
2:B:69:GLU:O	2:B:73:ILE:HG13	2.17	0.45
1:D:90:GLU:H	1:D:90:GLU:CD	2.19	0.45
3:E:570:SRM:HBA1	3:E:570:SRM:CHB	2.44	0.45
2:E:220:CYS:HA	2:E:221:PRO:HD3	1.82	0.45
1:D:290:HIS:HB2	2:E:275:ALA:HB1	1.99	0.45
1:A:361:ILE:HG23	1:A:362:GLY:N	2.32	0.45
2:E:40:VAL:HG22	2:E:54:VAL:HG13	1.99	0.45
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.83	0.45
1:D:339:GLU:OE2	1:D:379:ARG:NH2	2.41	0.44
2:B:4:GLU:HB3	2:B:5:GLY:H	1.64	0.44
1:A:208:TRP:HB3	1:A:209:PRO:HD2	1.99	0.44
1:A:387:LYS:N	2:B:357:GLU:O	2.49	0.44
2:B:237:ASP:C	2:B:237:ASP:OD1	2.56	0.44
2:E:55:ARG:NH2	3:E:570:SRM:HMB2	2.31	0.44
1:D:169:LEU:O	1:D:203:LEU:HG	2.17	0.44
1:A:42:LYS:HB2	1:A:42:LYS:HE3	1.51	0.44
1:D:170:ARG:O	1:D:172:PRO:HD3	2.17	0.44
1:D:250:LYS:O	1:D:253:ALA:N	2.39	0.44
1:A:168:ASP:OD2	1:A:203:LEU:O	2.35	0.43
2:E:183:GLY:O	2:E:186:HIS:CE1	2.71	0.43
2:E:44:VAL:HG13	2:E:48:GLY:HA2	2.00	0.43
2:E:135:GLN:O	2:E:138:ILE:HB	2.18	0.43
2:E:142:THR:HG22	2:E:248:TYR:HD2	1.83	0.43
2:E:248:TYR:CD1	2:E:255:PRO:HA	2.53	0.43
2:E:101:ASP:HA	2:E:104:ILE:HD12	1.99	0.43
2:E:316:LYS:O	2:E:317:HIS:CB	2.67	0.43
2:B:172:ARG:HH21	3:B:570:SRM:C2C	2.31	0.43
1:D:286:VAL:CB	2:E:363:GLN:HG3	2.49	0.43
1:D:169:LEU:O	1:D:203:LEU:HA	2.17	0.43
1:D:67:ILE:HG13	1:D:67:ILE:H	1.68	0.43
1:A:261:GLU:OE1	1:A:294:LYS:NZ	2.48	0.43
1:D:96:THR:HG22	1:D:139:LEU:HA	2.01	0.43
1:D:8:GLU:HG2	1:D:11:LYS:HZ2	1.82	0.43
1:A:393:PRO:HG3	2:E:181:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ALA:CB	2:E:272:LEU:HD21	2.48	0.43
1:A:217:ALA:HB1	1:A:222:ASP:HA	2.01	0.43
1:D:7:ASP:O	1:D:10:GLU:HB2	2.18	0.43
1:A:105:TRP:HD1	1:A:130:HIS:CD2	2.37	0.43
1:A:64:HIS:CE1	2:B:249:THR:O	2.71	0.43
2:E:253:GLY:C	2:E:255:PRO:HD3	2.39	0.43
1:D:222:ASP:OD1	1:D:227:LYS:HG2	2.19	0.43
1:D:262:VAL:O	1:D:263:VAL:C	2.58	0.42
1:A:371:ARG:CG	1:A:372:GLU:N	2.81	0.42
2:E:213:ILE:N	2:E:214:PRO:HD2	2.35	0.42
1:A:297:LYS:HE2	2:B:32:TYR:CD1	2.54	0.42
1:D:31:ALA:HB1	1:D:36:LYS:HB2	2.00	0.42
3:B:570:SRM:HHA	3:B:570:SRM:O4D	2.20	0.42
1:D:114:GLY:O	1:D:117:ASP:HB2	2.19	0.42
1:D:177:GLY:HA3	1:D:178:PRO:HD2	1.85	0.42
1:A:32:ALA:HB2	1:A:38:VAL:HB	2.00	0.42
1:D:228:ALA:CB	2:E:272:LEU:CD2	2.97	0.42
2:E:288:TRP:CH2	2:E:290:PRO:HB3	2.55	0.42
1:A:317:PHE:CE2	2:B:180:ASN:OD1	2.73	0.42
1:D:374:LEU:O	1:D:378:GLY:N	2.53	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.01	0.42
1:D:370:MET:O	1:D:374:LEU:HG	2.20	0.42
1:D:193:TYR:O	1:D:197:MET:HG2	2.19	0.42
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.01	0.42
1:D:408:THR:HA	1:D:411:LEU:HD12	2.01	0.42
1:A:28:MET:HE2	1:A:123:GLY:O	2.19	0.42
1:A:98:ARG:NH2	3:A:580:SRM:HMB3	2.34	0.41
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.50	0.41
2:E:269:GLY:O	2:E:321:ILE:HB	2.20	0.41
2:E:303:VAL:O	2:E:307:LEU:HB2	2.20	0.41
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.93	0.41
1:D:93:HIS:HB3	1:D:95:HIS:NE2	2.35	0.41
1:A:229:ARG:HG3	3:A:580:SRM:O4C	2.21	0.41
2:E:56:PHE:HD2	2:E:114:PRO:O	2.04	0.41
3:B:570:SRM:HHA	3:B:570:SRM:CED	2.50	0.41
1:A:129:PHE:HA	1:A:130:HIS:HA	1.80	0.41
1:A:407:TYR:OH	2:E:199:PRO:O	2.30	0.41
1:D:344:LEU:HB3	1:D:348:TRP:CH2	2.56	0.41
2:B:324:VAL:HG11	2:B:329:TRP:CZ2	2.55	0.41
1:A:178:PRO:HG3	1:A:187:ASP:HA	2.02	0.41
1:A:358:ARG:NH2	3:A:580:SRM:O3D	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ALA:HB1	2:E:181:MET:HA	2.03	0.41
2:E:135:GLN:HB3	2:E:139:HIS:HB3	2.02	0.41
2:B:324:VAL:HG11	2:B:329:TRP:CE2	2.56	0.41
1:D:132:SER:N	3:D:580:SRM:HBB1	2.36	0.40
1:A:315:ALA:HB3	3:A:580:SRM:HBD1	2.03	0.40
1:A:211:LYS:HZ1	3:A:580:SRM:HAD1	1.84	0.40
2:E:87:ARG:O	2:E:130:ASN:HB3	2.19	0.40
1:D:97:MET:HB2	1:D:138:PHE:HB2	2.02	0.40
1:A:128:ASN:HB2	1:A:137:ILE:CG1	2.51	0.40
1:D:96:THR:HG23	2:E:139:HIS:CE1	2.57	0.40
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	2.03	0.40
2:E:142:THR:O	2:E:178:CYS:SG	2.79	0.40
2:B:106:GLU:HG2	2:B:110:ARG:HD3	2.03	0.40
1:D:350:TRP:CG	1:D:376:VAL:HG21	2.56	0.40
2:B:323:TRP:O	2:B:327:ILE:HG12	2.21	0.40
2:E:121:ALA:CB	3:E:570:SRM:O3D	2.52	0.40
3:A:580:SRM:O3B	2:B:135:GLN:HG2	2.22	0.40
1:D:8:GLU:HG2	1:D:11:LYS:NZ	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	415/418 (99%)	392 (94%)	22 (5%)	1 (0%)	52	64
1	D	415/418 (99%)	380 (92%)	28 (7%)	7 (2%)	11	10
2	B	361/366 (99%)	331 (92%)	27 (8%)	3 (1%)	24	27
2	E	361/366 (99%)	308 (85%)	39 (11%)	14 (4%)	4	2
All	All	1552/1568 (99%)	1411 (91%)	116 (8%)	25 (2%)	12	11

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	251	GLU
2	E	6	VAL
2	E	160	GLU
2	E	231	ASN
1	D	250	LYS
2	E	79	ASP
2	E	122	VAL
2	E	5	GLY
2	E	45	ALA
2	E	135	GLN
2	E	332	PHE
1	A	69	SER
2	B	11	GLY
1	D	67	ILE
1	D	220	PRO
1	D	388	ALA
2	E	38	PRO
2	B	60	ARG
1	D	247	GLU
2	E	119	TRP
1	D	289	MET
2	E	60	ARG
2	E	143	PRO
2	E	208	ARG
2	B	142	THR

5.3.2 Protein sidechains ⓘ

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	353/354 (100%)	331 (94%)	22 (6%)	23	30
1	D	353/354 (100%)	332 (94%)	21 (6%)	24	32
2	B	314/317 (99%)	297 (95%)	17 (5%)	27	36
2	E	314/317 (99%)	290 (92%)	24 (8%)	16	20
All	All	1334/1342 (99%)	1250 (94%)	84 (6%)	22	29

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	42	LYS
1	A	48	LEU
1	A	50	GLN
1	A	86	GLU
1	A	92	GLU
1	A	94	PHE
1	A	100	ASN
1	A	133	THR
1	A	143	SER
1	A	224	VAL
1	A	229	ARG
1	A	295	MET
1	A	310	LEU
1	A	322	VAL
1	A	375	LYS
1	A	400	ASP
1	A	402	LEU
1	A	403	LYS
1	A	410	GLU
1	A	411	LEU
1	A	417	TRP
2	B	4	GLU
2	B	31	LYS
2	B	97	GLU
2	B	108	GLN
2	B	174	SER
2	B	189	ASP
2	B	205	GLU
2	B	230	LYS
2	B	235	LYS
2	B	242	MET
2	B	243	TYR
2	B	256	LEU
2	B	283	LYS
2	B	299	LEU
2	B	321	ILE
2	B	349	ARG
2	B	361	SER
1	D	42	LYS
1	D	54	SER
1	D	56	LYS

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Mol	Chain	Res	Type
1	D	90	GLU
1	D	98	ARG
1	D	100	ASN
1	D	133	THR
1	D	139	LEU
1	D	157	GLU
1	D	159	PRO
1	D	207	MET
1	D	210	TYR
1	D	213	LYS
1	D	234	ILE
1	D	241	ASP
1	D	254	SER
1	D	272	LYS
1	D	276	LYS
1	D	279	THR
1	D	334	GLU
1	D	413	LYS
2	E	4	GLU
2	E	46	GLU
2	E	51	ILE
2	E	58	THR
2	E	61	LEU
2	E	96	ASP
2	E	97	GLU
2	E	123	LYS
2	E	128	LEU
2	E	140	CYS
2	E	188	SER
2	E	205	GLU
2	E	210	THR
2	E	212	GLU
2	E	230	LYS
2	E	231	ASN
2	E	242	MET
2	E	243	TYR
2	E	267	MET
2	E	271	LYS
2	E	273	SER
2	E	307	LEU
2	E	335	LEU
2	E	345	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	100	ASN
1	A	147	GLN
2	B	108	GLN
2	B	139	HIS
1	D	100	ASN
1	D	282	ASN
2	E	180	ASN
2	E	363	GLN

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 13 ligands modelled in this entry, 1 is modelled with single atom - leaving 12 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	$\# Z > 2$
4	SF4	A	575	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	576	1	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SRM	A	580	2,5	29,70,70	2.08	7 (24%)	29,112,112	3.86	15 (51%)
3	SRM	B	570	1	29,70,70	2.71	9 (31%)	29,112,112	4.55	18 (62%)
4	SF4	B	585	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	586	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	575	1,6	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	576	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SRM	D	580	-	29,70,70	2.13	7 (24%)	29,112,112	4.25	13 (44%)
3	SRM	E	570	1	29,70,70	2.89	9 (31%)	29,112,112	5.35	15 (51%)
4	SF4	E	585	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	586	2	0,12,12	0.00	-	0,24,24	0.00	-

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
4	SF4	A	575	1	-	0/0/48/48	0/6/5/5
4	SF4	A	576	1	-	0/0/48/48	0/6/5/5
3	SRM	A	580	2,5	-	0/22/126/126	0/0/8/8
3	SRM	B	570	1	-	0/22/126/126	0/0/8/8
4	SF4	B	585	2	-	0/0/48/48	0/6/5/5
4	SF4	B	586	2	-	0/0/48/48	0/6/5/5
4	SF4	D	575	1,6	-	0/0/48/48	0/6/5/5
4	SF4	D	576	1	-	0/0/48/48	0/6/5/5
3	SRM	D	580	-	-	0/22/126/126	0/0/8/8
3	SRM	E	570	1	-	0/22/126/126	0/0/8/8
4	SF4	E	585	2	-	0/0/48/48	0/6/5/5
4	SF4	E	586	2	-	0/0/48/48	0/6/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4C-NC	-7.19	1.27	1.36
3	E	570	SRM	C1C-NC	-6.14	1.28	1.36
3	B	570	SRM	C4A-NA	-5.89	1.28	1.39
3	E	570	SRM	C4A-NA	-5.79	1.28	1.39
3	E	570	SRM	C1B-NB	-5.50	1.29	1.38
3	B	570	SRM	C1B-NB	-5.12	1.30	1.38
3	B	570	SRM	C4C-NC	-4.86	1.30	1.36
3	B	570	SRM	C1C-NC	-4.60	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	580	SRM	C4A-NA	-3.23	1.33	1.39
3	A	580	SRM	C4A-NA	-3.13	1.33	1.39
3	D	580	SRM	C1A-NA	-2.87	1.33	1.38
3	A	580	SRM	C1C-NC	-2.80	1.32	1.36
3	E	570	SRM	C1A-NA	-2.63	1.34	1.38
3	E	570	SRM	CHC-C4B	-2.29	1.34	1.39
3	E	570	SRM	C4B-NB	-2.14	1.35	1.39
3	B	570	SRM	C1D-CHD	-2.02	1.34	1.39
3	B	570	SRM	CAD-C2D	2.61	1.56	1.52
3	B	570	SRM	CAA-C3A	2.62	1.56	1.51
3	D	580	SRM	CAD-C2D	2.66	1.56	1.52
3	A	580	SRM	CAD-C2D	2.88	1.57	1.52
3	D	580	SRM	FE-NA	3.33	2.08	1.95
3	A	580	SRM	FE-NB	3.51	2.09	1.95
3	A	580	SRM	C3C-C2C	3.58	1.48	1.37
3	D	580	SRM	FE-NB	3.62	2.10	1.95
3	A	580	SRM	FE-NA	4.12	2.12	1.95
3	D	580	SRM	C3C-C2C	4.20	1.50	1.37
3	B	570	SRM	C3C-C2C	4.68	1.51	1.37
3	E	570	SRM	C3C-C2C	4.90	1.52	1.37
3	E	570	SRM	C3D-C2D	5.71	1.52	1.39
3	A	580	SRM	C3D-C2D	6.55	1.54	1.39
3	D	580	SRM	C3D-C2D	6.57	1.54	1.39
3	B	570	SRM	C3D-C2D	6.99	1.55	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-13.56	108.19	123.46
3	B	570	SRM	CAA-C3A-C2A	-12.75	109.11	123.46
3	E	570	SRM	CAD-C2D-C1D	-12.08	113.89	127.01
3	D	580	SRM	CAB-C3B-C2B	-11.39	110.64	123.46
3	E	570	SRM	CDC-C2C-C1C	-10.87	109.84	127.38
3	E	570	SRM	CDD-C3D-C4D	-10.55	110.20	127.34
3	E	570	SRM	CAA-C3A-C2A	-10.14	112.05	123.46
3	E	570	SRM	CAC-C3C-C4C	-9.93	116.22	127.01
3	D	580	SRM	CDD-C3D-C4D	-9.89	111.26	127.34
3	B	570	SRM	CAD-C2D-C1D	-9.26	116.95	127.01
3	D	580	SRM	CAD-C2D-C1D	-8.83	117.42	127.01
3	A	580	SRM	CDD-C3D-C4D	-6.83	116.24	127.34
3	E	570	SRM	C4A-NA-C1A	-6.79	103.21	106.90
3	E	570	SRM	CAD-C2D-C3D	-6.40	113.45	129.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CEC-CDC-C2C	-6.38	104.12	116.31
3	D	580	SRM	CAA-C3A-C2A	-6.23	116.45	123.46
3	A	580	SRM	CAD-C2D-C3D	-5.91	114.66	129.38
3	B	570	SRM	C4A-NA-C1A	-5.87	103.72	106.90
3	A	580	SRM	CAA-C3A-C2A	-5.73	117.01	123.46
3	B	570	SRM	CDD-C3D-C4D	-5.46	118.47	127.34
3	E	570	SRM	CAC-C3C-C2C	-5.12	116.64	129.38
3	B	570	SRM	CAC-C3C-C2C	-5.05	116.81	129.38
3	B	570	SRM	CBC-CAC-C3C	-5.00	103.56	112.53
3	B	570	SRM	CMA-C2A-CDA	-4.65	104.23	109.76
3	E	570	SRM	CMA-C2A-CDA	-4.56	104.34	109.76
3	D	580	SRM	CAD-C2D-C3D	-4.00	119.44	129.38
3	D	580	SRM	C4B-NB-C1B	-3.47	105.02	106.90
3	B	570	SRM	CDC-C2C-C1C	-3.44	121.82	127.38
3	E	570	SRM	CHB-C4A-C3A	-3.33	117.90	125.48
3	E	570	SRM	CBC-CAC-C3C	-3.17	106.85	112.53
3	B	570	SRM	CHB-C4A-C3A	-3.10	118.43	125.48
3	A	580	SRM	CAD-C2D-C1D	-3.07	123.67	127.01
3	A	580	SRM	CAC-CBC-CCC	-2.53	108.12	112.75
3	E	570	SRM	CEC-CDC-C2C	-2.52	111.49	116.31
3	D	580	SRM	C3A-C4A-NA	-2.37	107.45	110.09
3	D	580	SRM	C2B-CDB-CEB	-2.24	111.98	115.45
3	B	570	SRM	CAC-C3C-C4C	-2.08	124.75	127.01
3	A	580	SRM	CMA-C2A-CDA	2.01	112.16	109.76
3	A	580	SRM	CHB-C4A-C3A	2.04	130.11	125.48
3	D	580	SRM	CDC-C2C-C1C	2.07	130.73	127.38
3	B	570	SRM	CHC-C4B-NB	2.11	127.82	123.70
3	A	580	SRM	C3B-C4B-NB	2.26	112.60	110.09
3	A	580	SRM	CAC-C3C-C4C	2.53	129.75	127.01
3	D	580	SRM	C3B-C4B-NB	2.55	112.92	110.09
3	B	570	SRM	CED-CDD-C3D	2.73	121.52	116.31
3	E	570	SRM	CAA-CBA-CCA	2.81	117.90	112.75
3	E	570	SRM	C2B-CDB-CEB	3.05	120.17	115.45
3	A	580	SRM	C2A-CDA-CEA	3.30	120.56	115.45
3	A	580	SRM	CBC-CAC-C3C	3.51	118.82	112.53
3	B	570	SRM	C2B-CDB-CEB	3.70	121.19	115.45
3	A	580	SRM	CDC-C2C-C1C	3.95	133.75	127.38
3	B	570	SRM	CAB-CBB-CCB	3.96	120.00	112.75
3	A	580	SRM	CBD-CAD-C2D	4.02	119.73	112.53
3	B	570	SRM	CAA-CBA-CCA	4.05	120.16	112.75
3	D	580	SRM	CBD-CAD-C2D	4.54	120.67	112.53
3	A	580	SRM	C4A-NA-C1A	4.98	109.61	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	570	SRM	CBD-CAD-C2D	6.22	123.67	112.53
3	B	570	SRM	C3A-C4A-NA	6.27	117.06	110.09
3	D	580	SRM	CMA-C2A-CDA	6.35	117.32	109.76
3	E	570	SRM	C3A-C4A-NA	7.31	118.22	110.09
3	D	580	SRM	C4A-NA-C1A	7.56	111.00	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	580	SRM	24	0
3	B	570	SRM	7	0
4	B	585	SF4	2	0
4	D	575	SF4	1	0
3	D	580	SRM	13	0
3	E	570	SRM	13	0
4	E	585	SF4	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, 95th 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	417/418 (99%)	0.39	15 (3%) 46 55	3, 7, 15, 31	0
1	D	417/418 (99%)	1.55	116 (27%) 1 1	2, 7, 13, 19	0
2	B	363/366 (99%)	0.23	4 (1%) 82 86	2, 6, 11, 20	0
2	E	363/366 (99%)	1.61	102 (28%) 1 1	2, 5, 23, 40	0
All	All	1560/1568 (99%)	0.95	237 (15%) 3 5	2, 6, 15, 40	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	231	ASN	8.7
1	D	40	MET	8.7
1	D	81	TYR	8.3
2	E	229	MET	8.2
1	D	87	GLN	7.5
1	D	1	SER	6.9
1	D	94	PHE	6.5
1	D	106	PHE	6.5
1	D	67	ILE	6.4
2	E	230	LYS	6.4
2	E	210	THR	6.1
1	D	12	GLY	6.0
2	E	236	VAL	5.7
2	E	82	LEU	5.6
1	D	91	VAL	5.3
2	E	4	GLU	5.2
2	E	27	TYR	5.2
2	E	67	VAL	5.1
1	D	115	LEU	5.0
1	D	47	LEU	5.0
1	D	39	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
2	E	296	TRP	4.9
2	E	150	ILE	4.8
1	D	145	TYR	4.8
1	D	417	TRP	4.8
1	A	417	TRP	4.7
1	D	68	VAL	4.6
1	D	43	GLY	4.6
1	D	29	GLU	4.5
1	D	42	LYS	4.3
1	D	72	GLY	4.2
2	E	28	GLY	4.2
1	A	413	LYS	4.1
1	D	38	VAL	4.1
1	D	70	VAL	4.1
1	D	74	GLY	4.0
2	E	81	TYR	4.0
2	E	56	PHE	4.0
2	E	92	PHE	4.0
1	D	144	GLU	4.0
2	E	6	VAL	4.0
1	D	126	LEU	4.0
1	D	76	GLY	3.9
2	E	179	ALA	3.9
2	E	233	THR	3.9
1	D	65	GLY	3.9
1	D	24	THR	3.9
1	D	5	LEU	3.9
2	E	47	SER	3.8
1	D	136	ILE	3.8
2	E	70	LEU	3.8
1	D	31	ALA	3.8
1	D	147	GLN	3.7
2	E	51	ILE	3.7
1	D	33	ALA	3.6
2	E	227	PRO	3.6
1	D	160	PHE	3.6
2	E	57	GLY	3.6
1	D	99	ILE	3.6
2	E	109	GLU	3.6
1	D	41	PRO	3.5
1	D	273	TRP	3.5
2	E	36	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	132	SER	3.5
2	E	232	LYS	3.5
2	E	185	VAL	3.5
1	A	414	ARG	3.5
2	E	305	GLN	3.5
1	A	402	LEU	3.4
1	D	122	TRP	3.4
2	E	209	LYS	3.4
2	E	110	ARG	3.4
2	E	40	VAL	3.3
1	D	276	LYS	3.3
2	E	61	LEU	3.3
1	D	193	TYR	3.3
2	E	134	THR	3.2
1	D	32	ALA	3.2
1	D	84	LEU	3.2
1	D	207	MET	3.2
1	D	164	GLY	3.1
2	E	55	ARG	3.1
2	E	173	ILE	3.1
2	E	206	ALA	3.1
1	D	335	LYS	3.1
2	E	218	ALA	3.1
1	D	328	VAL	3.1
1	A	415	GLY	3.1
1	D	60	THR	3.1
2	E	41	ILE	3.0
2	B	5	GLY	3.0
1	D	108	SER	3.0
2	E	107	VAL	3.0
2	E	64	ILE	3.0
1	D	180	LEU	3.0
1	D	2	GLU	3.0
2	E	34	GLU	3.0
2	E	52	TYR	3.0
1	D	78	ILE	3.0
2	E	98	SER	3.0
1	D	30	LYS	3.0
1	D	49	LYS	2.9
2	E	235	LYS	2.9
1	D	85	GLY	2.9
2	E	50	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	62	TRP	2.9
1	D	45	ARG	2.9
2	E	256	LEU	2.9
1	D	105	TRP	2.9
2	E	30	TRP	2.9
1	D	77	VAL	2.8
1	D	244	VAL	2.8
1	D	263	VAL	2.8
2	E	207	ILE	2.8
2	E	208	ARG	2.8
1	D	242	ILE	2.8
2	E	15	PHE	2.8
1	D	28	MET	2.8
2	E	77	TYR	2.8
1	D	83	ASP	2.8
1	D	157	GLU	2.8
1	D	159	PRO	2.8
2	E	257	PHE	2.7
1	A	406	ALA	2.7
1	A	411	LEU	2.7
2	E	76	LYS	2.7
2	E	243	TYR	2.7
2	E	248	TYR	2.7
2	E	288	TRP	2.7
1	D	26	GLU	2.6
2	E	205	GLU	2.6
1	D	220	PRO	2.6
1	D	51	LEU	2.6
1	D	195	LEU	2.6
2	B	4	GLU	2.6
1	D	330	PHE	2.6
2	E	162	PHE	2.6
2	E	103	LEU	2.6
1	D	292	ILE	2.6
2	E	159	TYR	2.6
2	E	180	ASN	2.6
1	D	71	VAL	2.6
1	D	82	SER	2.6
2	E	144	ALA	2.6
2	E	239	GLU	2.5
1	D	120	GLU	2.5
1	D	181	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	254	SER	2.5
1	D	153	LEU	2.5
1	D	155	ASN	2.5
1	D	48	LEU	2.5
1	D	137	ILE	2.5
1	D	357	PHE	2.5
1	D	275	GLY	2.5
2	E	118	THR	2.5
2	E	111	VAL	2.5
1	D	127	THR	2.4
2	E	219	ALA	2.4
2	E	65	TYR	2.4
1	D	255	TRP	2.4
1	D	351	TRP	2.4
1	D	329	PRO	2.4
2	E	59	PRO	2.4
1	D	299	LEU	2.4
2	E	5	GLY	2.4
1	D	129	PHE	2.4
2	E	72	ASP	2.3
2	E	339	GLU	2.3
2	E	104	ILE	2.3
2	E	177	CYS	2.3
1	D	152	ASP	2.3
2	B	227	PRO	2.3
2	E	96	ASP	2.3
2	E	112	GLY	2.3
1	D	57	ASP	2.3
2	E	94	VAL	2.3
2	E	293	PRO	2.3
1	D	141	THR	2.3
1	D	315	ALA	2.3
1	D	123	GLY	2.3
1	A	416	MET	2.3
1	D	6	LEU	2.3
1	D	107	TYR	2.3
1	D	112	LEU	2.3
2	E	90	VAL	2.3
1	D	317	PHE	2.3
1	D	109	THR	2.2
1	A	285	CYS	2.2
1	D	11	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	17	PHE	2.2
1	D	150	PHE	2.2
2	E	311	ALA	2.2
1	A	67	ILE	2.2
1	D	73	TYR	2.2
2	E	115	CYS	2.2
2	E	220	CYS	2.2
2	E	333	PHE	2.2
2	E	272	LEU	2.2
2	E	42	LYS	2.2
2	E	84	TRP	2.2
1	A	412	LYS	2.2
1	A	398	GLU	2.2
1	D	334	GLU	2.2
1	D	117	ASP	2.2
2	E	199	PRO	2.2
2	E	312	ALA	2.2
2	E	68	ARG	2.1
1	D	178	PRO	2.1
2	E	8	THR	2.1
1	D	253	ALA	2.1
2	E	137	TRP	2.1
2	E	158	LEU	2.1
1	D	50	GLN	2.1
2	E	187	ALA	2.1
2	E	73	ILE	2.1
2	E	18	LEU	2.1
1	D	179	ALA	2.1
2	E	337	GLY	2.1
2	E	255	PRO	2.1
2	E	37	LYS	2.1
1	A	400	ASP	2.1
1	D	15	PRO	2.1
1	D	175	CYS	2.0
2	E	178	CYS	2.0
2	E	181	MET	2.0
2	B	236	VAL	2.0
2	E	286	VAL	2.0
1	D	305	ARG	2.0
2	E	16	ARG	2.0
1	D	35	GLY	2.0
1	D	218	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	249	VAL	2.0
2	E	154	VAL	2.0
1	A	409	GLU	2.0
1	D	284	GLU	2.0
1	D	191	LEU	2.0
1	A	407	TYR	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, 95th 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
3	SRM	D	580	63/63	0.84	0.28	1.25	18,21,24,30	0
3	SRM	E	570	63/63	0.92	0.24	0.56	5,5,6,6	0
3	SRM	A	580	63/63	0.95	0.13	-0.41	7,10,14,17	0
3	SRM	B	570	63/63	0.95	0.13	-0.63	3,4,6,7	0
4	SF4	E	585	8/8	0.95	0.13	-1.80	19,20,21,21	0
4	SF4	E	586	8/8	0.96	0.06	-2.38	13,15,15,16	0
4	SF4	D	576	8/8	0.93	0.08	-2.62	7,7,8,8	0
4	SF4	B	586	8/8	0.98	0.06	-2.64	2,3,3,3	0
4	SF4	A	576	8/8	0.97	0.06	-3.09	5,6,6,6	0
4	SF4	B	585	8/8	0.97	0.05	-3.52	10,11,12,16	0
4	SF4	D	575	8/8	0.95	0.10	-3.56	3,3,3,3	0
4	SF4	A	575	8/8	0.98	0.07	-4.34	6,6,7,7	0
5	H2S	A	590	1/1	0.92	0.11	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.