



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 03:52 PM EDT

PDB ID : 5EUL
Title : Structure of the SecA-SecY complex with a translocating polypeptide substrate
Authors : Li, L.; Park, E.; Ling, J.; Ingram, J.; Ploegh, H.; Rapoport, T.A.
Deposited on : 2015-11-18
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

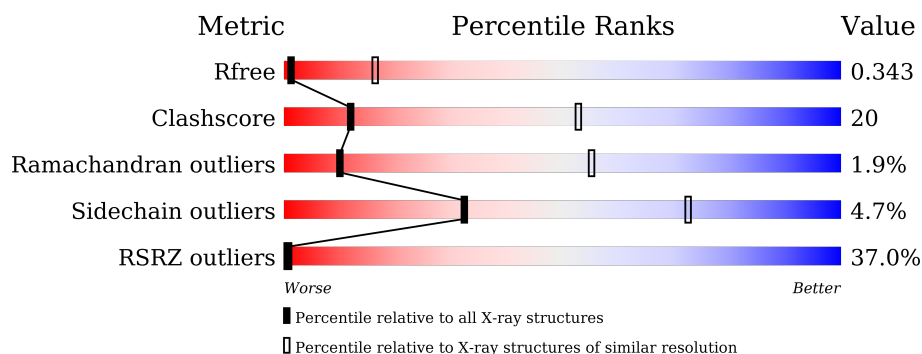
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	836	<div> <div>36%</div> <div>60%</div> <div>25%</div> <div>11%</div> </div>
2	Y	424	<div> <div>30%</div> <div>49%</div> <div>35%</div> <div>10%</div> </div>
3	E	70	<div> <div>29%</div> <div>56%</div> <div>23%</div> <div>20%</div> </div>
4	V	131	<div> <div>24%</div> <div>54%</div> <div>29%</div> <div>12%</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
8	TBR	A	1014	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10511 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 Protein translocase subunit SecA, Insertion Peptide Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			5876	3677	1030	1135	34			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	THR	-	expression tag	UNP P28366
A	829	SER	-	expression tag	UNP P28366
A	830	LEU	-	expression tag	UNP P28366
A	831	GLU	-	expression tag	UNP P28366
A	832	VAL	-	expression tag	UNP P28366
A	833	LEU	-	expression tag	UNP P28366
A	834	PHE	-	expression tag	UNP P28366
A	835	GLN	-	expression tag	UNP P28366
A	836	GLY	-	expression tag	UNP P28366

- Molecule 2 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	380	Total	C	N	O	S	0	0	0
			2936	1951	478	495	12			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	60	CYS	GLY	conflict	UNP A4IJK8
Y	208	THR	GLN	conflict	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8
Y	?	-	ASN	deletion	UNP A4IJK8
Y	?	-	VAL	deletion	UNP A4IJK8
Y	?	-	GLY	deletion	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ASP	deletion	UNP A4IJK8
Y	210	GLY	LEU	conflict	UNP A4IJK8
Y	211	GLY	PHE	conflict	UNP A4IJK8
Y	213	ASN	ARG	conflict	UNP A4IJK8

- Molecule 3 is a protein called Preprotein translocase SecE subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	56	Total	C	N	O	0	0	0
			460	306	78	76			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLY	-	expression tag	UNP A4IJH4
E	62	GLY	-	expression tag	UNP A4IJH4
E	63	HIS	-	expression tag	UNP A4IJH4
E	64	HIS	-	expression tag	UNP A4IJH4
E	65	HIS	-	expression tag	UNP A4IJH4
E	66	HIS	-	expression tag	UNP A4IJH4
E	67	HIS	-	expression tag	UNP A4IJH4
E	68	HIS	-	expression tag	UNP A4IJH4
E	69	HIS	-	expression tag	UNP A4IJH4
E	70	HIS	-	expression tag	UNP A4IJH4

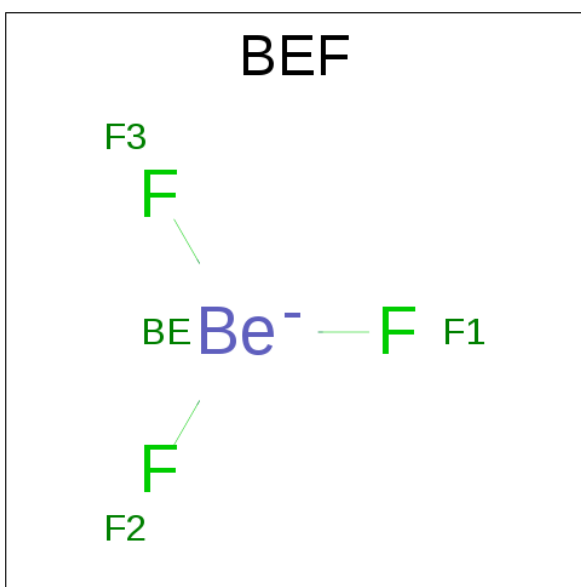
- Molecule 4 is a protein called AYC08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	V	115	Total	C	N	O	S	0	0	0
			883	553	153	171	6			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

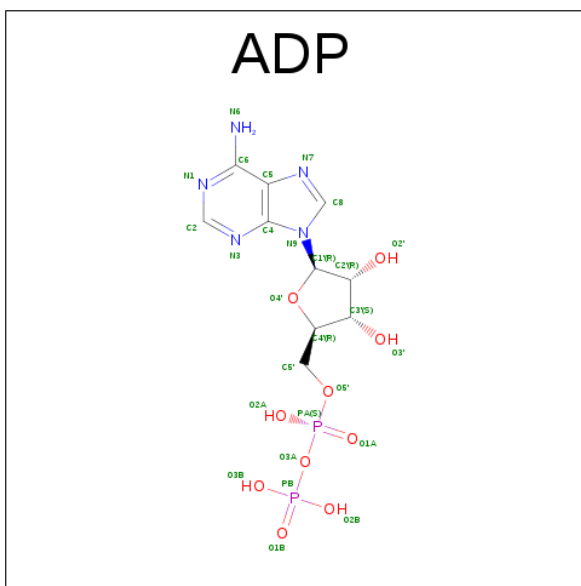
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



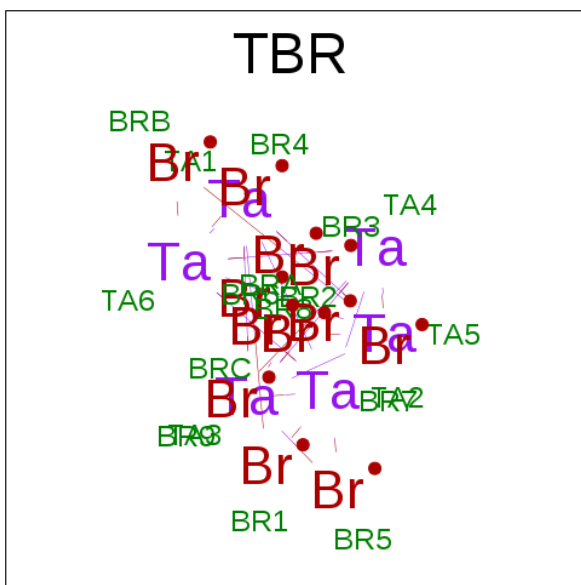
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Be	F	0	0
			4	1	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

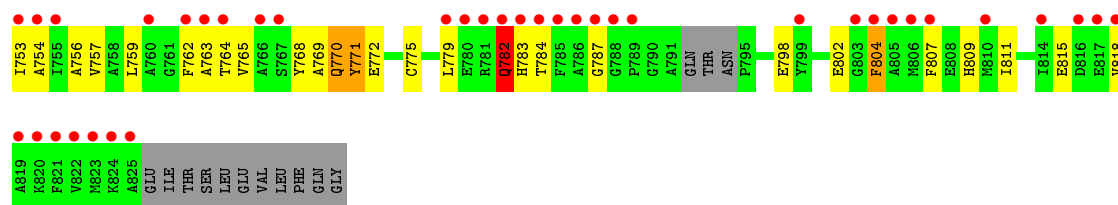
- Molecule 8 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $\text{Br}_{12}\text{Ta}_6$).

[illegible]

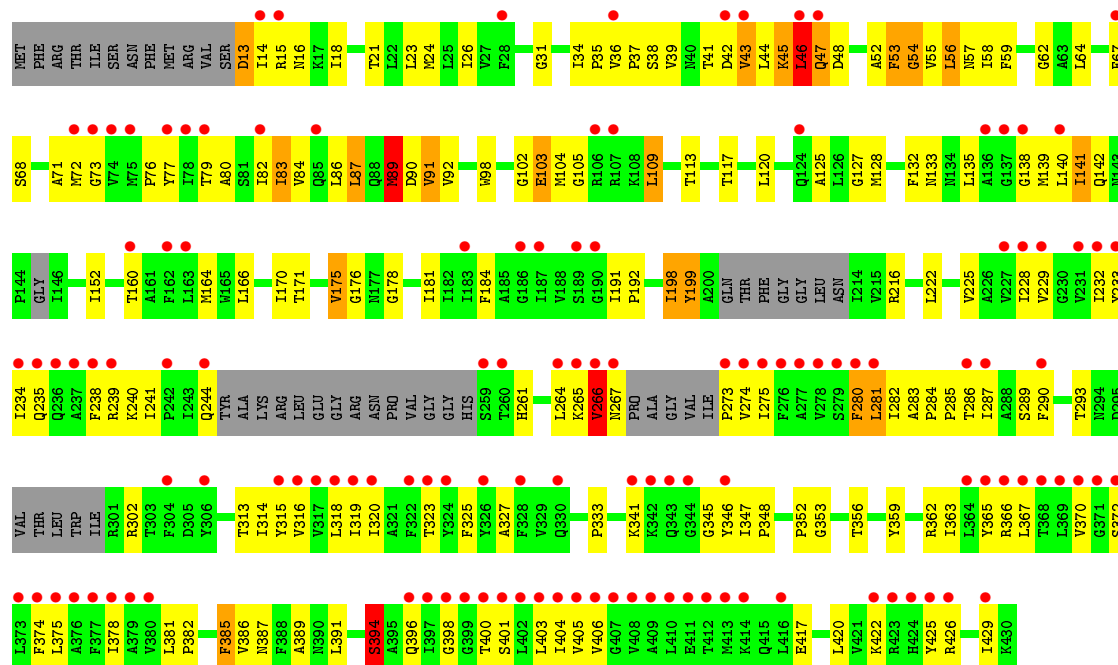
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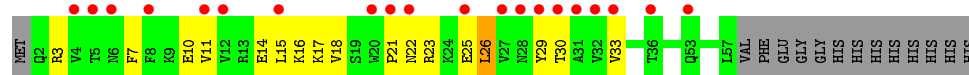
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0



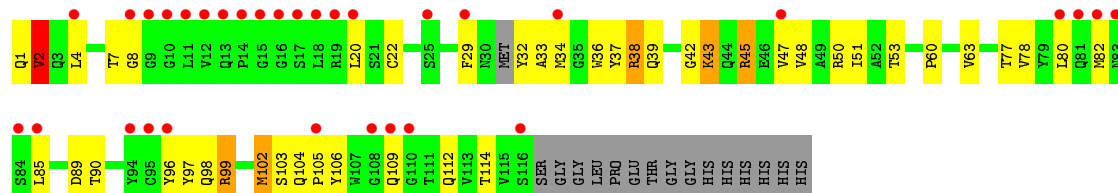
• Molecule 2: Protein translocase subunit SecY



• Molecule 3: Preprotein translocase SecE subunit



• Molecule 4: AYC08



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.80 Å 127.80 Å 554.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.85 – 3.70 110.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.85-3.70) 99.9 (110.68-3.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.67 Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.318 , 0.343	Depositor DCC
R_{free} test set	1509 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	191.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 172.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	3 of 29882 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	10511	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TBR, BEF, ADP

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	0.29	1/5950 (0.0%)	0.55	2/7993 (0.0%)
2	Y	0.37	0/2996	0.68	3/4069 (0.1%)
3	E	0.31	0/469	0.52	0/635
4	V	0.29	0/901	0.67	1/1222 (0.1%)
All	All	0.32	1/10316 (0.0%)	0.60	6/13919 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
2	Y	0	8
4	V	0	3
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	804	PHE	CB-CG	-5.07	1.42	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	46	LEU	CA-CB-CG	7.64	132.87	115.30
4	V	43	LYS	N-CA-C	6.37	128.19	111.00
1	A	804	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	256	THR	N-CA-C	5.74	126.50	111.00
2	Y	89	MET	C-N-CA	5.55	135.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	109	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ALA	Peptide
1	A	229	LYS	Peptide
1	A	242	ARG	Peptide
1	A	243	THR	Peptide
1	A	244	LEU	Peptide
1	A	255	LYS	Peptide
1	A	410	THR	Peptide
1	A	451	ASN	Peptide
1	A	452	LYS	Peptide
1	A	461	ALA	Peptide
1	A	563	MET	Peptide
1	A	768	TYR	Peptide
1	A	770	GLN	Peptide
1	A	782	GLN	Peptide
4	V	102	MET	Peptide
4	V	42	GLY	Peptide
4	V	43	LYS	Peptide
2	Y	138	GLY	Peptide
2	Y	198	ILE	Peptide
2	Y	266	VAL	Peptide
2	Y	394	SER	Peptide
2	Y	425	TYR	Peptide
2	Y	46	LEU	Peptide
2	Y	54	GLY	Peptide
2	Y	89	MET	Peptide

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	5876	0	5855	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2936	0	3075	187	0
3	E	460	0	482	26	0
4	V	883	0	845	38	0
5	A	1	0	0	0	0
6	A	4	0	0	1	0
7	A	27	0	12	1	0
8	A	270	0	0	28	0
8	Y	54	0	0	2	0
All	All	10511	0	10269	416	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 20.

All (416) 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)
2:Y:265:LYS:HG3	2:Y:266:VAL:HG23	1.42	1.00
1:A:242:ARG:HH22	1:A:268:LYS:HB3	1.30	0.94
2:Y:229:VAL:HG12	3:E:30:THR:HG21	1.52	0.92
2:Y:24:MET:HB3	2:Y:166:LEU:HD21	1.51	0.90
2:Y:235:GLN:HG3	2:Y:266:VAL:HG22	1.55	0.88
1:A:242:ARG:CZ	1:A:265:GLY:HA2	2.04	0.88
1:A:241:VAL:HG12	1:A:242:ARG:H	1.40	0.86
2:Y:91:VAL:HG23	2:Y:92:VAL:H	1.41	0.85
2:Y:239:ARG:NH2	3:E:14:GLU:O	2.12	0.83
1:A:188:ASN:O	1:A:614:ARG:NH1	2.11	0.82
1:A:550:GLY:HA2	1:A:581:SER:HB3	1.64	0.80
1:A:240:PHE:HZ	1:A:242:ARG:HH21	1.27	0.79
1:A:120:THR:HG21	8:A:1009:TBR:BR1	2.38	0.78
2:Y:370:VAL:HG21	3:E:15:LEU:HD11	1.66	0.78
4:V:4:LEU:O	4:V:109:GLN:NE2	2.18	0.76
8:A:1012:TBR:BRA	2:Y:289:SER:OG	2.58	0.76
2:Y:346:TYR:HB3	2:Y:352:PRO:HG3	1.69	0.75
2:Y:386:VAL:HA	2:Y:389:ALA:HB2	1.67	0.75
1:A:410:THR:O	1:A:412:GLU:N	2.16	0.75
1:A:422:VAL:HG12	1:A:432:VAL:HG11	1.69	0.74
2:Y:14:ILE:O	2:Y:18:ILE:HG13	1.87	0.74
1:A:753:ILE:HD12	2:Y:86:LEU:HG	1.70	0.74
1:A:302:LYS:O	1:A:304:VAL:N	2.21	0.73
1:A:74:ARG:HD3	8:A:1016:TBR:BR8	2.43	0.72
2:Y:366:ARG:CZ	3:E:10:GLU:HB3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:39:GLN:HB2	4:V:45:ARG:HB3	1.72	0.72
1:A:240:PHE:HZ	1:A:242:ARG:NH2	1.87	0.71
1:A:461:ALA:HA	1:A:464:HIS:HB3	1.71	0.71
1:A:254:ILE:HA	1:A:548:ARG:HB3	1.72	0.71
1:A:782:GLN:O	1:A:784:THR:N	2.20	0.71
1:A:261:LEU:HD22	2:Y:341:LYS:HZ3	1.56	0.71
2:Y:366:ARG:HB3	3:E:11:VAL:HA	1.72	0.71
1:A:459:LEU:HD22	1:A:486:MET:HG3	1.74	0.70
4:V:32:TYR:O	4:V:53:THR:OG1	2.08	0.70
2:Y:362:ARG:HH21	2:Y:366:ARG:HH22	1.39	0.70
2:Y:273:PRO:HB3	2:Y:327:ALA:HB2	1.73	0.70
3:E:3:ARG:HB3	3:E:7:PHE:HE2	1.57	0.69
1:A:459:LEU:HD11	1:A:467:GLU:HG3	1.75	0.69
2:Y:265:LYS:CG	2:Y:266:VAL:HG23	2.22	0.69
1:A:804:PHE:HA	2:Y:426:ARG:HH21	1.59	0.68
1:A:301:GLN:HG3	1:A:302:LYS:H	1.59	0.68
2:Y:281:LEU:HD21	2:Y:315:TYR:CZ	2.30	0.67
2:Y:43:VAL:HB	2:Y:140:LEU:HD12	1.75	0.67
1:A:787:GLY:H	2:Y:275:ILE:HG21	1.60	0.67
2:Y:86:LEU:HD21	2:Y:280:PHE:HZ	1.59	0.66
2:Y:46:LEU:HA	4:V:45:ARG:HH21	1.59	0.66
1:A:81:PRO:HG3	1:A:108:LEU:HD11	1.77	0.66
1:A:523:ARG:NH1	1:A:535:THR:OG1	2.28	0.66
1:A:92:LEU:HD21	1:A:370:MET:HG2	1.77	0.66
1:A:322:ARG:HA	1:A:461:ALA:HB2	1.78	0.66
1:A:540:SER:N	1:A:543:ASP:OD1	2.28	0.65
1:A:804:PHE:HA	2:Y:426:ARG:NH2	2.12	0.65
2:Y:139:MET:HE1	4:V:47:VAL:HB	1.78	0.65
1:A:439:VAL:HG12	1:A:460:ASN:HD21	1.61	0.65
2:Y:378:ILE:HG21	2:Y:403:LEU:HD11	1.78	0.65
1:A:457:GLN:OE1	1:A:466:ARG:NH1	2.30	0.64
4:V:33:ALA:N	4:V:98:GLN:O	2.27	0.64
2:Y:281:LEU:HD22	2:Y:319:ILE:HG12	1.78	0.64
2:Y:80:ALA:HB3	2:Y:117:THR:HG22	1.80	0.64
1:A:542:GLU:HG3	1:A:547:ARG:NE	2.13	0.63
1:A:630:MET:SD	1:A:818:VAL:HG21	2.39	0.63
1:A:555:MET:O	1:A:559:ASP:N	2.29	0.63
2:Y:46:LEU:HA	4:V:45:ARG:NH2	2.13	0.63
1:A:266:MET:HG2	1:A:279:PHE:CZ	2.34	0.63
2:Y:225:VAL:HA	2:Y:228:ILE:HG12	1.81	0.63
1:A:304:VAL:HG23	1:A:305:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG11	1:A:369:GLY:HA3	1.81	0.62
4:V:32:TYR:HA	4:V:99:ARG:HA	1.80	0.62
2:Y:86:LEU:HD21	2:Y:280:PHE:CZ	2.35	0.62
1:A:394:THR:O	1:A:395:ASN:HB3	2.00	0.62
1:A:228:ALA:HB2	1:A:348:GLU:H	1.66	0.61
2:Y:239:ARG:HD3	2:Y:241:ILE:HD11	1.81	0.61
1:A:301:GLN:HG3	1:A:302:LYS:N	2.14	0.61
1:A:606:GLN:HE21	2:Y:426:ARG:NH2	1.99	0.61
4:V:1:GLN:O	4:V:2:VAL:HG13	2.00	0.60
1:A:335:GLN:HE22	1:A:348:GLU:HG2	1.65	0.60
1:A:544:GLU:OE1	8:A:1006:TBR:BRC	2.74	0.60
2:Y:323:THR:HG21	2:Y:372:SER:HA	1.83	0.60
1:A:550:GLY:HA2	1:A:581:SER:CB	2.29	0.60
2:Y:175:VAL:HG12	2:Y:176:GLY:H	1.65	0.60
1:A:802:GLU:HB2	8:A:1005:TBR:BR2	2.57	0.60
2:Y:102:GLY:O	2:Y:104:MET:N	2.35	0.60
2:Y:232:ILE:HG21	3:E:30:THR:HG23	1.84	0.60
2:Y:281:LEU:HD11	2:Y:315:TYR:CD1	2.37	0.60
2:Y:400:THR:HA	2:Y:403:LEU:HD12	1.85	0.59
2:Y:52:ALA:O	2:Y:53:PHE:HB2	2.02	0.59
1:A:595:GLN:HB2	8:A:1004:TBR:BR2	2.57	0.59
1:A:228:ALA:HB1	1:A:230:SER:HB3	1.85	0.59
1:A:264:GLU:O	1:A:268:LYS:HB2	2.02	0.59
1:A:545:LEU:O	1:A:550:GLY:N	2.35	0.58
8:A:1017:TBR:BR7	2:Y:104:MET:SD	3.16	0.58
1:A:359:ASN:ND2	1:A:600:ASP:OD1	2.37	0.58
1:A:770:GLN:HE22	2:Y:293:THR:HG21	1.68	0.58
2:Y:286:THR:HA	2:Y:289:SER:HB3	1.86	0.57
2:Y:37:PRO:O	2:Y:142:GLN:NE2	2.38	0.57
1:A:254:ILE:HA	1:A:548:ARG:CB	2.34	0.57
1:A:759:LEU:HD13	2:Y:284:PRO:HG3	1.87	0.57
2:Y:239:ARG:NH2	3:E:14:GLU:HG3	2.20	0.57
2:Y:239:ARG:HB3	2:Y:264:LEU:HB2	1.86	0.57
2:Y:285:PRO:O	2:Y:289:SER:HB2	2.04	0.57
1:A:309:GLU:HG2	8:A:1014:TBR:BR8	2.60	0.56
1:A:738:ILE:HD11	1:A:798:GLU:HB3	1.86	0.56
2:Y:113:THR:O	2:Y:117:THR:HG23	2.04	0.56
2:Y:235:GLN:HG3	2:Y:266:VAL:CG2	2.34	0.56
1:A:309:GLU:HG3	8:A:1014:TBR:BR7	2.61	0.56
3:E:30:THR:HA	3:E:33:VAL:HG12	1.87	0.56
1:A:439:VAL:HG12	1:A:460:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:GLY:N	2:Y:275:ILE:HG21	2.20	0.56
1:A:421:ASP:OD2	1:A:425:ARG:NE	2.38	0.56
2:Y:44:LEU:HD13	2:Y:56:LEU:HA	1.88	0.56
1:A:156:LEU:HB2	1:A:159:MET:HG3	1.88	0.56
2:Y:72:MET:HE2	2:Y:125:ALA:HB2	1.88	0.55
1:A:453:GLY:O	1:A:454:ILE:HG13	2.06	0.55
2:Y:198:ILE:HG23	2:Y:199:TYR:H	1.70	0.55
2:Y:46:LEU:HD11	4:V:47:VAL:HG22	1.88	0.55
3:E:22:ASN:HB3	3:E:25:GLU:CB	2.36	0.55
1:A:36:LEU:HG	1:A:40:ALA:HB3	1.89	0.55
1:A:82:PHE:HB2	1:A:85:GLN:HG3	1.89	0.55
1:A:236:GLN:HB3	1:A:273:PHE:HE1	1.71	0.55
1:A:450:LYS:HD3	8:A:1015:TBR:BRA	2.62	0.55
1:A:304:VAL:HG23	1:A:305:ASP:N	2.22	0.55
1:A:253:ASP:O	1:A:548:ARG:HG2	2.07	0.55
1:A:590:PHE:CE2	2:Y:103:GLU:HG2	2.41	0.55
2:Y:389:ALA:HB1	2:Y:391:LEU:HB2	1.89	0.55
1:A:433:LEU:HD21	1:A:525:ARG:CZ	2.38	0.54
1:A:544:GLU:OE1	8:A:1006:TBR:BR4	2.81	0.54
1:A:779:LEU:HD11	2:Y:62:GLY:HA3	1.87	0.54
1:A:377:GLU:OE2	1:A:517:ARG:NH1	2.41	0.54
1:A:561:PHE:HZ	1:A:569:ILE:HG21	1.72	0.54
4:V:22:CYS:O	4:V:77:THR:HA	2.08	0.54
1:A:418:VAL:HG23	1:A:508:VAL:HG11	1.90	0.54
2:Y:366:ARG:HB2	3:E:14:GLU:HG2	1.89	0.54
1:A:242:ARG:NH2	1:A:265:GLY:HA2	2.22	0.54
2:Y:68:SER:H	2:Y:71:ALA:HB2	1.73	0.54
2:Y:385:PHE:O	2:Y:389:ALA:HB2	2.08	0.53
2:Y:417:GLU:HA	2:Y:420:LEU:HB3	1.90	0.53
2:Y:41:THR:HG22	2:Y:45:LYS:NZ	2.23	0.53
2:Y:238:PHE:HE1	2:Y:265:LYS:HE2	1.73	0.53
4:V:22:CYS:HB3	4:V:78:VAL:HG22	1.91	0.53
3:E:22:ASN:HB3	3:E:25:GLU:HB2	1.90	0.53
4:V:99:ARG:NH2	4:V:102:MET:O	2.37	0.53
1:A:753:ILE:HD11	2:Y:325:PHE:HZ	1.74	0.52
2:Y:286:THR:O	2:Y:290:PHE:N	2.42	0.52
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.90	0.52
1:A:242:ARG:NH2	1:A:265:GLY:O	2.42	0.52
2:Y:225:VAL:O	2:Y:229:VAL:HG13	2.10	0.52
1:A:187:ASP:OD2	1:A:197:VAL:HG22	2.09	0.52
2:Y:44:LEU:HD11	2:Y:67:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:SD	1:A:352:LEU:HD22	2.50	0.52
2:Y:273:PRO:HB3	2:Y:327:ALA:CB	2.39	0.52
2:Y:45:LYS:HZ1	2:Y:55:VAL:HG23	1.74	0.52
4:V:36:TRP:O	4:V:48:VAL:N	2.33	0.51
1:A:261:LEU:CD2	2:Y:341:LYS:HZ3	2.21	0.51
1:A:203:PHE:HD1	1:A:204:ALA:N	2.08	0.51
1:A:335:GLN:NE2	1:A:348:GLU:HG2	2.25	0.51
1:A:240:PHE:CZ	1:A:242:ARG:NH2	2.73	0.51
2:Y:35:PRO:HB3	2:Y:56:LEU:HD21	1.92	0.51
1:A:317:ASP:HB3	1:A:320:THR:OG1	2.10	0.51
1:A:693:ILE:HG23	8:A:1010:TBR:BR7	2.65	0.51
2:Y:16:ASN:HD22	2:Y:16:ASN:N	2.09	0.51
1:A:630:MET:CE	2:Y:429:ILE:HA	2.40	0.51
1:A:192:TYR:HB2	1:A:195:GLN:HG2	1.93	0.51
1:A:14:ARG:NH1	8:A:1018:TBR:BR1	2.99	0.50
1:A:348:GLU:OE2	8:A:1013:TBR:BR2	2.84	0.50
4:V:20:LEU:HD12	4:V:80:LEU:HD23	1.93	0.50
2:Y:387:ASN:C	2:Y:389:ALA:H	2.14	0.50
1:A:285:ALA:HB1	8:A:1013:TBR:BR4	2.66	0.50
1:A:614:ARG:HG3	1:A:720:VAL:HG11	1.93	0.50
2:Y:315:TYR:O	2:Y:319:ILE:HG13	2.11	0.50
2:Y:353:GLY:O	2:Y:356:THR:OG1	2.25	0.50
2:Y:239:ARG:NH2	3:E:18:VAL:HG23	2.25	0.50
1:A:233:LEU:HB3	1:A:236:GLN:HB2	1.94	0.50
1:A:242:ARG:NH2	1:A:268:LYS:HB3	2.12	0.50
1:A:542:GLU:HG3	1:A:547:ARG:HE	1.77	0.50
3:E:15:LEU:O	3:E:18:VAL:HB	2.12	0.50
2:Y:283:ALA:HB3	2:Y:284:PRO:HD3	1.94	0.50
1:A:770:GLN:NE2	2:Y:293:THR:HG21	2.25	0.50
2:Y:267:ASN:HA	2:Y:367:LEU:HD11	1.94	0.50
2:Y:36:VAL:CG1	2:Y:152:ILE:HG13	2.42	0.50
2:Y:91:VAL:HG23	2:Y:92:VAL:N	2.19	0.50
1:A:807:PHE:CE2	1:A:811:ILE:HD11	2.47	0.49
1:A:261:LEU:HD13	2:Y:341:LYS:NZ	2.28	0.49
1:A:756:ALA:HB1	2:Y:280:PHE:HE2	1.77	0.49
1:A:564:ASP:O	1:A:565:ASP:HB2	2.11	0.49
1:A:724:TRP:CE2	1:A:728:ILE:HD11	2.48	0.49
3:E:3:ARG:HB3	3:E:7:PHE:CE2	2.43	0.49
4:V:48:VAL:HG13	4:V:63:VAL:HG21	1.94	0.49
2:Y:38:SER:CB	2:Y:152:ILE:HG12	2.42	0.49
2:Y:21:THR:HA	2:Y:170:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLN:C	1:A:784:THR:H	2.13	0.49
1:A:266:MET:HG2	1:A:279:PHE:HZ	1.78	0.49
1:A:436:THR:HG22	1:A:437:VAL:H	1.77	0.49
1:A:409:ARG:HH21	1:A:564:ASP:H	1.61	0.49
4:V:109:GLN:H	4:V:109:GLN:CD	2.15	0.49
2:Y:13:ASP:N	2:Y:13:ASP:OD2	2.45	0.49
4:V:37:TYR:HD2	4:V:96:TYR:HD2	1.59	0.49
1:A:409:ARG:HG2	1:A:410:THR:H	1.77	0.49
1:A:549:PHE:CD1	1:A:585:VAL:HG22	2.48	0.49
4:V:34:MET:HE2	4:V:78:VAL:HG11	1.95	0.49
2:Y:43:VAL:HB	2:Y:140:LEU:CD1	2.42	0.49
2:Y:244:GLN:O	2:Y:345:GLY:HA3	2.13	0.49
2:Y:54:GLY:HA3	2:Y:57:ASN:HB2	1.93	0.49
1:A:262:THR:C	1:A:265:GLY:H	2.17	0.48
2:Y:362:ARG:HH21	2:Y:366:ARG:NH2	2.10	0.48
1:A:809:HIS:CE1	8:A:1011:TBR:BRB	3.21	0.48
2:Y:98:TRP:CE3	2:Y:109:LEU:HD13	2.48	0.48
2:Y:281:LEU:HD21	2:Y:315:TYR:CE1	2.48	0.48
2:Y:31:GLY:HA2	2:Y:34:ILE:HD13	1.94	0.48
1:A:242:ARG:HH22	1:A:268:LYS:CB	2.13	0.48
4:V:29:PHE:HE1	4:V:34:MET:HG3	1.79	0.48
1:A:242:ARG:HH12	1:A:268:LYS:HE2	1.78	0.48
4:V:34:MET:HB2	4:V:51:ILE:HG23	1.95	0.48
1:A:223:ILE:O	1:A:352:LEU:HB2	2.14	0.48
2:Y:45:LYS:C	2:Y:47:GLN:H	2.17	0.48
1:A:284:VAL:C	1:A:286:LEU:H	2.17	0.48
1:A:281:VAL:HG13	2:Y:348:PRO:HB3	1.95	0.48
2:Y:36:VAL:HB	2:Y:39:VAL:HG13	1.95	0.48
1:A:811:ILE:O	1:A:815:GLU:HG3	2.14	0.47
2:Y:42:ASP:OD2	4:V:50:ARG:NE	2.45	0.47
2:Y:14:ILE:HG13	2:Y:15:ARG:N	2.29	0.47
1:A:302:LYS:HD3	8:A:1007:TBR:BR3	2.69	0.47
1:A:763:ALA:HB2	2:Y:283:ALA:HA	1.96	0.47
2:Y:241:ILE:HG22	2:Y:347:ILE:HD12	1.96	0.47
4:V:48:VAL:O	4:V:60:PRO:HD2	2.15	0.47
3:E:25:GLU:HG2	3:E:29:TYR:CD2	2.50	0.47
2:Y:58:ILE:HD11	2:Y:132:PHE:HZ	1.80	0.47
2:Y:86:LEU:O	2:Y:89:MET:HG2	2.14	0.47
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.68	0.47
1:A:292:GLN:NE2	1:A:331:GLU:O	2.48	0.47
2:Y:235:GLN:HA	2:Y:266:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG12	2:Y:346:TYR:OH	2.15	0.47
1:A:709:ARG:O	1:A:712:GLU:HG2	2.15	0.46
2:Y:232:ILE:CD1	3:E:29:TYR:HB3	2.45	0.46
2:Y:320:ILE:HA	2:Y:372:SER:OG	2.14	0.46
1:A:443:GLU:HB2	8:A:1007:TBR:BRC	2.71	0.46
4:V:37:TYR:HA	4:V:48:VAL:HG23	1.96	0.46
1:A:259:VAL:HG22	1:A:260:GLN:H	1.80	0.46
1:A:242:ARG:HH12	1:A:268:LYS:CE	2.29	0.46
1:A:84:VAL:HG11	1:A:395:ASN:HB2	1.98	0.46
2:Y:240:LYS:HD2	2:Y:261:HIS:CE1	2.51	0.46
2:Y:91:VAL:HG23	2:Y:92:VAL:HG12	1.98	0.46
1:A:254:ILE:HA	1:A:548:ARG:CA	2.45	0.46
2:Y:82:ILE:O	2:Y:86:LEU:HD13	2.16	0.46
2:Y:382:PRO:HD3	2:Y:398:GLY:O	2.15	0.46
2:Y:45:LYS:HG3	2:Y:48:ASP:OD1	2.15	0.46
2:Y:56:LEU:HB3	2:Y:67:PHE:O	2.16	0.46
8:A:1012:TBR:BR5	2:Y:289:SER:OG	2.84	0.46
1:A:73:SER:OG	1:A:108:LEU:HD21	2.16	0.46
1:A:301:GLN:CG	1:A:302:LYS:H	2.29	0.46
1:A:630:MET:HE3	2:Y:429:ILE:HA	1.98	0.46
2:Y:386:VAL:CA	2:Y:389:ALA:HB2	2.42	0.46
1:A:115:TYR:CE2	1:A:119:LEU:HD21	2.52	0.45
4:V:82:MET:HB3	4:V:85:LEU:HD11	1.98	0.45
2:Y:417:GLU:OE1	8:Y:502:TBR:BR9	2.89	0.45
1:A:105:GLY:O	1:A:109:THR:HG23	2.16	0.45
1:A:302:LYS:O	1:A:303:ASP:C	2.52	0.45
1:A:304:VAL:CG2	1:A:305:ASP:H	2.27	0.45
2:Y:362:ARG:HE	2:Y:366:ARG:CZ	2.29	0.45
1:A:630:MET:HE3	2:Y:429:ILE:HG23	1.97	0.45
1:A:108:LEU:O	1:A:111:THR:HG22	2.17	0.45
1:A:233:LEU:HD13	1:A:236:GLN:OE1	2.16	0.45
1:A:275:ILE:HB	1:A:283:HIS:CE1	2.52	0.45
1:A:487:ALA:HA	1:A:525:ARG:CZ	2.47	0.45
4:V:29:PHE:HE1	4:V:34:MET:SD	2.39	0.45
4:V:29:PHE:CE1	4:V:34:MET:SD	3.10	0.45
2:Y:375:LEU:O	2:Y:378:ILE:HG22	2.16	0.45
1:A:804:PHE:HE1	8:Y:502:TBR:BR2	2.55	0.45
1:A:100:MET:O	1:A:106:LYS:HE2	2.17	0.45
3:E:22:ASN:CG	3:E:23:ARG:H	2.20	0.45
1:A:464:HIS:NE2	8:A:1014:TBR:BRC	3.04	0.45
2:Y:102:GLY:C	2:Y:105:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:381:LEU:N	2:Y:382:PRO:HD2	2.32	0.45
2:Y:362:ARG:NH2	2:Y:366:ARG:HH22	2.11	0.45
1:A:329:TYR:HB3	1:A:333:LEU:HB3	1.97	0.44
1:A:561:PHE:HZ	1:A:569:ILE:CG2	2.29	0.44
1:A:769:ALA:HA	2:Y:127:GLY:O	2.17	0.44
2:Y:191:ILE:N	2:Y:192:PRO:HD2	2.32	0.44
1:A:242:ARG:HG2	1:A:243:THR:N	2.32	0.44
1:A:86:LEU:O	1:A:90:VAL:HG23	2.18	0.44
2:Y:133:ASN:HD21	2:Y:141:ILE:HG12	1.82	0.44
2:Y:238:PHE:O	3:E:18:VAL:HG13	2.17	0.44
1:A:625:GLU:HG3	8:A:1010:TBR:BR9	2.72	0.44
1:A:26:ILE:HG12	1:A:63:VAL:HA	1.98	0.44
1:A:753:ILE:HG13	2:Y:89:MET:SD	2.56	0.44
4:V:109:GLN:H	4:V:109:GLN:NE2	2.15	0.44
1:A:242:ARG:HG2	1:A:244:LEU:N	2.32	0.44
1:A:322:ARG:HA	1:A:461:ALA:CB	2.47	0.44
4:V:82:MET:CB	4:V:85:LEU:HD11	2.48	0.44
1:A:311:GLY:O	1:A:343:LEU:HD13	2.17	0.44
2:Y:14:ILE:O	2:Y:18:ILE:N	2.49	0.44
2:Y:239:ARG:HB3	2:Y:264:LEU:CB	2.47	0.44
1:A:762:PHE:HB2	2:Y:287:ILE:HD11	1.99	0.44
2:Y:46:LEU:HD23	4:V:105:PRO:HG3	1.99	0.44
2:Y:54:GLY:HA3	2:Y:57:ASN:CB	2.48	0.44
1:A:313:VAL:HG11	1:A:337:ILE:HG22	2.00	0.44
2:Y:15:ARG:HA	2:Y:18:ILE:HD12	1.99	0.44
2:Y:62:GLY:HA2	2:Y:394:SER:HA	1.99	0.44
2:Y:166:LEU:O	2:Y:170:ILE:HG22	2.17	0.44
1:A:303:ASP:HA	1:A:306:TYR:O	2.17	0.44
1:A:33:TYR:O	1:A:36:LEU:HB2	2.18	0.44
1:A:764:THR:HG23	1:A:765:VAL:HG23	2.00	0.44
1:A:266:MET:HG2	1:A:279:PHE:CE2	2.52	0.43
1:A:302:LYS:HE2	1:A:308:VAL:CG2	2.48	0.43
2:Y:160:THR:O	2:Y:164:MET:N	2.47	0.43
1:A:130:ASN:HB2	1:A:322:ARG:NH1	2.32	0.43
1:A:546:MET:SD	1:A:578:VAL:HG22	2.57	0.43
2:Y:313:THR:HA	2:Y:316:VAL:HG12	1.99	0.43
2:Y:45:LYS:HE2	2:Y:45:LYS:HB2	1.89	0.43
2:Y:45:LYS:NZ	2:Y:56:LEU:H	2.16	0.43
4:V:90:THR:HG23	4:V:114:THR:HA	1.99	0.43
4:V:34:MET:O	4:V:50:ARG:HA	2.17	0.43
2:Y:275:ILE:HG12	2:Y:404:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:O	1:A:298:VAL:HG22	2.19	0.43
1:A:590:PHE:HE2	2:Y:103:GLU:HG2	1.82	0.43
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.79	0.43
1:A:242:ARG:HG2	1:A:244:LEU:H	1.83	0.43
1:A:295:LYS:O	1:A:299:ALA:HB3	2.19	0.43
1:A:749:LYS:HG2	1:A:750:LYS:H	1.83	0.43
3:E:22:ASN:HB3	3:E:25:GLU:HB3	2.00	0.43
2:Y:184:PHE:HD1	2:Y:405:VAL:HA	1.84	0.43
1:A:214:ILE:HG21	1:A:377:GLU:OE1	2.19	0.43
4:V:38:ARG:NH2	4:V:89:ASP:HA	2.34	0.43
2:Y:103:GLU:HA	2:Y:103:GLU:OE1	2.18	0.43
1:A:256:THR:HB	1:A:548:ARG:NH2	2.33	0.43
1:A:301:GLN:HA	1:A:301:GLN:HE21	1.83	0.43
1:A:321:GLY:HA3	1:A:485:ASN:HB2	2.01	0.43
2:Y:387:ASN:C	2:Y:389:ALA:N	2.72	0.43
2:Y:239:ARG:HA	3:E:18:VAL:HG22	2.01	0.42
2:Y:79:THR:HG23	2:Y:120:LEU:HD13	2.00	0.42
2:Y:140:LEU:HA	2:Y:140:LEU:HD23	1.72	0.42
2:Y:396:GLN:HG3	2:Y:401:SER:OG	2.19	0.42
4:V:7:THR:OG1	4:V:8:GLY:N	2.52	0.42
1:A:771:TYR:HE1	2:Y:135:LEU:HD22	1.84	0.42
2:Y:84:VAL:HA	2:Y:87:LEU:HB2	2.00	0.42
1:A:197:VAL:HG23	1:A:198:GLN:N	2.35	0.42
1:A:421:ASP:O	1:A:425:ARG:HG3	2.19	0.42
1:A:750:LYS:O	1:A:751:THR:C	2.57	0.42
2:Y:229:VAL:HB	3:E:26:LEU:HD11	2.00	0.42
2:Y:128:MET:O	2:Y:132:PHE:HB2	2.20	0.42
2:Y:76:PRO:HA	2:Y:79:THR:HG22	2.01	0.42
1:A:99:GLU:HA	1:A:371:THR:O	2.18	0.42
1:A:422:VAL:HG21	1:A:449:LEU:HD21	2.00	0.42
1:A:85:GLN:HB3	1:A:109:THR:HG22	2.01	0.42
1:A:241:VAL:HG12	1:A:242:ARG:N	2.22	0.42
1:A:493:ILE:HD12	1:A:505:LEU:HD21	2.01	0.42
1:A:770:GLN:HB3	1:A:772:GLU:HG3	2.00	0.42
3:E:25:GLU:OE2	3:E:29:TYR:HE2	2.02	0.42
4:V:97:TYR:CE2	4:V:106:TYR:HB3	2.54	0.42
1:A:244:LEU:HD13	1:A:250:TYR:N	2.35	0.42
1:A:288:HIS:CE1	1:A:292:GLN:HE21	2.37	0.42
1:A:807:PHE:O	1:A:811:ILE:HG13	2.20	0.42
2:Y:234:ILE:HG13	2:Y:374:PHE:CE1	2.54	0.42
2:Y:386:VAL:HA	2:Y:389:ALA:CB	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:48:ASP:HA	2:Y:58:ILE:HG23	2.02	0.42
2:Y:79:THR:HA	2:Y:82:ILE:HG22	2.01	0.42
1:A:586:GLU:HB3	8:A:1017:TBR:BR5	2.74	0.42
1:A:115:TYR:O	1:A:119:LEU:HD22	2.19	0.42
1:A:302:LYS:HE2	1:A:308:VAL:HG21	2.02	0.42
1:A:581:SER:O	1:A:585:VAL:HG23	2.19	0.42
1:A:582:GLN:HA	1:A:585:VAL:HG23	2.01	0.42
1:A:757:VAL:HG21	2:Y:87:LEU:HD12	2.02	0.42
1:A:275:ILE:HD12	1:A:278:LEU:HA	2.02	0.42
1:A:751:THR:HG22	1:A:754:ALA:H	1.85	0.42
2:Y:267:ASN:HA	2:Y:367:LEU:CD1	2.49	0.42
2:Y:370:VAL:HG21	3:E:15:LEU:CD1	2.42	0.42
2:Y:422:LYS:O	2:Y:426:ARG:HB2	2.20	0.42
2:Y:170:ILE:HG23	2:Y:178:GLY:HA3	2.02	0.42
2:Y:178:GLY:HA2	2:Y:181:ILE:HG12	2.01	0.42
1:A:410:THR:OG1	1:A:542:GLU:HB2	2.20	0.41
1:A:77:THR:HG23	1:A:79:MET:H	1.84	0.41
2:Y:59:PHE:CE2	2:Y:64:LEU:HD11	2.55	0.41
1:A:52:LEU:HD13	1:A:120:THR:HG23	2.02	0.41
1:A:600:ASP:O	1:A:604:ARG:N	2.46	0.41
1:A:259:VAL:HG11	2:Y:341:LYS:HG2	2.02	0.41
1:A:325:LYS:HE2	8:A:1014:TBR:BR4	2.75	0.41
1:A:688:ILE:O	1:A:692:ILE:HG13	2.19	0.41
2:Y:45:LYS:C	2:Y:47:GLN:N	2.73	0.41
2:Y:83:ILE:HG23	2:Y:87:LEU:HD13	2.03	0.41
1:A:313:VAL:HG23	1:A:334:HIS:NE2	2.35	0.41
1:A:303:ASP:HB3	1:A:439:VAL:CG2	2.51	0.41
6:A:1002:BEF:F2	7:A:1003:ADP:O1B	2.28	0.41
1:A:693:ILE:HD13	8:A:1010:TBR:BRB	2.76	0.41
2:Y:73:GLY:O	2:Y:76:PRO:HD2	2.21	0.41
1:A:47:GLU:HA	8:A:1008:TBR:BR8	2.76	0.41
1:A:458:VAL:HG11	8:A:1015:TBR:BR4	2.76	0.41
1:A:84:VAL:CG1	1:A:395:ASN:HB2	2.50	0.41
2:Y:171:THR:HB	2:Y:178:GLY:H	1.86	0.41
1:A:252:TYR:CG	1:A:255:LYS:HB2	2.56	0.41
1:A:690:ASP:HA	1:A:693:ILE:HD12	2.02	0.41
1:A:630:MET:HG3	1:A:815:GLU:HG2	2.03	0.41
2:Y:314:ILE:O	2:Y:318:LEU:HG	2.20	0.41
2:Y:406:VAL:HG12	3:E:33:VAL:HG21	2.01	0.41
2:Y:41:THR:HG22	2:Y:45:LYS:HZ3	1.85	0.41
2:Y:77:TYR:HA	2:Y:117:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:16:LYS:O	3:E:16:LYS:HD2	2.21	0.41
4:V:38:ARG:H	4:V:38:ARG:HG2	1.67	0.41
4:V:99:ARG:NH2	4:V:103:SER:O	2.54	0.41
2:Y:98:TRP:HE3	2:Y:109:LEU:HD13	1.86	0.41
2:Y:139:MET:HE3	2:Y:140:LEU:HG	2.02	0.41
2:Y:36:VAL:HG12	2:Y:38:SER:H	1.86	0.41
2:Y:229:VAL:O	2:Y:232:ILE:HG22	2.21	0.40
2:Y:389:ALA:HB1	2:Y:391:LEU:CB	2.50	0.40
1:A:458:VAL:HG11	8:A:1015:TBR:BRC	2.77	0.40
1:A:211:SER:HA	1:A:215:ASP:HB2	2.03	0.40
1:A:725:MET:HB3	1:A:725:MET:HE3	1.91	0.40
1:A:775:CYS:HB2	2:Y:135:LEU:HD13	2.02	0.40
4:V:36:TRP:CG	4:V:80:LEU:HD22	2.55	0.40
2:Y:184:PHE:HE1	2:Y:405:VAL:HG13	1.87	0.40
2:Y:282:ILE:O	2:Y:285:PRO:HG2	2.22	0.40
1:A:464:HIS:CD2	8:A:1014:TBR:BRC	3.29	0.40
2:Y:198:ILE:CG2	2:Y:199:TYR:H	2.33	0.40
1:A:495:LEU:HD23	1:A:528:ARG:HD2	2.03	0.40
1:A:753:ILE:HA	1:A:756:ALA:HB3	2.03	0.40
2:Y:222:LEU:O	2:Y:225:VAL:HG12	2.21	0.40
2:Y:359:TYR:O	2:Y:363:ILE:HD13	2.22	0.40
1:A:549:PHE:HD1	1:A:585:VAL:HG22	1.83	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	730/836 (87%)	676 (93%)	42 (6%)	12 (2%)	12 58
2	Y	368/424 (87%)	335 (91%)	24 (6%)	9 (2%)	7 51
3	E	54/70 (77%)	49 (91%)	4 (7%)	1 (2%)	10 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	111/131 (85%)	99 (89%)	10 (9%)	2 (2%)	11	56
All	All	1263/1461 (86%)	1159 (92%)	80 (6%)	24 (2%)	10	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	411	MET
1	A	452	LYS
1	A	782	GLN
1	A	783	HIS
2	Y	266	VAL
1	A	241	VAL
1	A	242	ARG
1	A	303	ASP
2	Y	90	ASP
2	Y	91	VAL
4	V	2	VAL
1	A	244	LEU
1	A	302	LYS
2	Y	103	GLU
1	A	485	ASN
1	A	565	ASP
2	Y	274	VAL
2	Y	46	LEU
2	Y	53	PHE
2	Y	175	VAL
3	E	21	PRO
4	V	104	GLN
2	Y	333	PRO

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	622/706 (88%)	598 (96%)	24 (4%)	39	76
2	Y	313/354 (88%)	293 (94%)	20 (6%)	22	64
3	E	50/63 (79%)	48 (96%)	2 (4%)	38	76
4	V	93/108 (86%)	88 (95%)	5 (5%)	27	69
All	All	1078/1231 (88%)	1027 (95%)	51 (5%)	32	72

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	59	ASP
1	A	70	ARG
1	A	119	LEU
1	A	203	PHE
1	A	207	ASP
1	A	208	GLU
1	A	209	VAL
1	A	251	THR
1	A	252	TYR
1	A	301	GLN
1	A	317	ASP
1	A	322	ARG
1	A	323	LEU
1	A	367	LEU
1	A	420	GLU
1	A	439	VAL
1	A	452	LYS
1	A	459	LEU
1	A	531	ASP
1	A	546	MET
1	A	561	PHE
1	A	735	ARG
1	A	771	TYR
2	Y	13	ASP
2	Y	23	LEU
2	Y	26	ILE
2	Y	43	VAL
2	Y	45	LYS
2	Y	46	LEU
2	Y	47	GLN
2	Y	56	LEU
2	Y	83	ILE

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Mol	Chain	Res	Type
2	Y	87	LEU
2	Y	141	ILE
2	Y	199	TYR
2	Y	216	ARG
2	Y	233	TYR
2	Y	280	PHE
2	Y	281	LEU
2	Y	302	ARG
2	Y	365	TYR
2	Y	385	PHE
2	Y	394	SER
3	E	17	LYS
3	E	26	LEU
4	V	2	VAL
4	V	38	ARG
4	V	45	ARG
4	V	99	ARG
4	V	112	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	125	HIS
1	A	140	GLN
1	A	292	GLN
1	A	301	GLN
1	A	347	ASN
1	A	383	ASN
1	A	598	GLN
1	A	605	GLN
1	A	613	GLN
1	A	629	ASN
1	A	739	HIS
2	Y	16	ASN
2	Y	66	ASN
2	Y	101	GLN
2	Y	124	GLN
2	Y	134	ASN
2	Y	169	GLN
2	Y	308	HIS
2	Y	335	GLN

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Mol	Chain	Res	Type
4	V	13	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
6	BEF	A	1002	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	A	1003	1,5,6	24,29,29	0.98	1 (4%)	23,45,45	1.74	1 (4%)
8	TBR	A	1004	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1005	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1006	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1007	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1008	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1009	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1010	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1011	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1012	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1013	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1014	-	0,36,36	0.00	-	0,180,180	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	TBR	A	1015	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1016	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1017	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1018	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	501	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	502	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	503	-	0,36,36	0.00	-	0,180,180	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
6	BEF	A	1002	7	-	0/0/0/0	0/0/0/0
7	ADP	A	1003	1,5,6	-	0/12/32/32	0/3/3/3
8	TBR	A	1004	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1005	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1006	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1007	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1008	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1009	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1010	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1011	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1012	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1013	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1014	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1015	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1016	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1017	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1018	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	501	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	502	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	503	-	-	0/0/696/696	0/0/19/19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1003	ADP	C5-C4	3.11	1.47	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	A	1003	ADP	N3-C2-N1	-6.57	123.71	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	BEF	1	0
7	A	1003	ADP	1	0
8	A	1004	TBR	1	0
8	A	1005	TBR	1	0
8	A	1006	TBR	2	0
8	A	1007	TBR	2	0
8	A	1008	TBR	1	0
8	A	1009	TBR	1	0
8	A	1010	TBR	3	0
8	A	1011	TBR	1	0
8	A	1012	TBR	2	0
8	A	1013	TBR	2	0
8	A	1014	TBR	5	0
8	A	1015	TBR	3	0
8	A	1016	TBR	1	0
8	A	1017	TBR	2	0
8	A	1018	TBR	1	0
8	Y	502	TBR	2	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	746/836 (89%)	1.91	301 (40%) 0 1	113, 202, 268, 329	0
2	Y	380/424 (89%)	1.71	127 (33%) 0 1	116, 191, 258, 282	0
3	E	56/70 (80%)	1.38	20 (35%) 0 1	155, 220, 261, 265	0
4	V	115/131 (87%)	1.73	32 (27%) 1 1	117, 166, 219, 253	2 (1%)
All	All	1297/1461 (88%)	1.81	480 (37%) 0 1	113, 196, 261, 329	2 (0%)

All (480) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	783	HIS	22.8
1	A	784	THR	15.4
1	A	823	MET	14.8
2	Y	267	ASN	14.8
2	Y	399	GLY	14.1
4	V	16	GLY	13.2
4	V	17	SER	13.0
2	Y	400	THR	12.9
2	Y	398	GLY	12.8
4	V	19	ARG	12.5
1	A	781	ARG	11.6
2	Y	401	SER	11.5
1	A	549	PHE	11.3
1	A	511	GLU	11.0
2	Y	396	GLN	10.7
1	A	512	ARG	10.2
1	A	785	PHE	10.0
1	A	819	ALA	9.8
1	A	541	MET	9.8
1	A	786	ALA	9.7
2	Y	273	PRO	9.4

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Mol	Chain	Res	Type	RSRZ
4	V	15	GLY	9.2
1	A	822	VAL	9.1
2	Y	276	PHE	8.7
1	A	514	GLU	8.5
1	A	440	GLU	8.4
2	Y	367	LEU	8.3
1	A	824	LYS	8.3
2	Y	366	ARG	8.3
2	Y	343	GLN	8.3
2	Y	275	ILE	8.1
1	A	354	THR	8.0
1	A	780	GLU	8.0
4	V	10	GLY	7.9
1	A	817	GLU	7.8
2	Y	236	GLN	7.8
2	Y	406	VAL	7.7
4	V	83	ASN	7.7
1	A	301	GLN	7.6
1	A	803	GLY	7.6
2	Y	365	TYR	7.5
2	Y	233	TYR	7.5
4	V	18	LEU	7.4
2	Y	397	ILE	7.4
1	A	546	MET	7.3
1	A	240	PHE	7.3
1	A	820	LYS	7.3
3	E	22	ASN	7.2
1	A	787	GLY	7.2
1	A	818	VAL	7.2
4	V	14	PRO	7.1
2	Y	266	VAL	7.1
2	Y	265	LYS	7.0
1	A	713	LYS	7.0
1	A	357	PHE	7.0
1	A	764	THR	7.0
2	Y	274	VAL	7.0
2	Y	371	GLY	7.0
4	V	9	GLY	6.9
2	Y	375	LEU	6.9
1	A	554	THR	6.9
2	Y	238	PHE	6.9
1	A	782	GLN	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	355	ILE	6.7
1	A	712	GLU	6.7
4	V	109	GLN	6.7
1	A	568	PRO	6.7
1	A	569	ILE	6.6
1	A	779	LEU	6.6
1	A	767	SER	6.6
1	A	253	ASP	6.6
2	Y	426	ARG	6.5
1	A	513	HIS	6.5
4	V	4	LEU	6.4
1	A	510	THR	6.4
2	Y	74	VAL	6.3
1	A	361	PHE	6.3
1	A	532	PRO	6.3
1	A	375	LYS	6.3
2	Y	235	GLN	6.2
1	A	821	PHE	6.2
4	V	96	TYR	6.2
1	A	398	VAL	6.2
1	A	407	ILE	6.1
4	V	105	PRO	6.1
1	A	319	PHE	6.1
4	V	8	GLY	6.1
1	A	708	MET	6.1
1	A	313	VAL	6.0
1	A	22	ILE	5.9
1	A	441	THR	5.9
2	Y	368	THR	5.9
1	A	432	VAL	5.9
2	Y	378	ILE	5.9
1	A	551	ALA	5.8
2	Y	319	ILE	5.7
2	Y	425	TYR	5.7
4	V	84	SER	5.7
3	E	11	VAL	5.7
1	A	374	ALA	5.7
1	A	273	PHE	5.7
2	Y	73	GLY	5.7
1	A	218	ARG	5.6
2	Y	279	SER	5.6
2	Y	423	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	694	THR	5.5
1	A	389	VAL	5.5
4	V	13	GLN	5.5
1	A	350	MET	5.5
4	V	11	LEU	5.4
1	A	224	SER	5.4
2	Y	402	LEU	5.4
1	A	437	VAL	5.4
1	A	260	GLN	5.4
1	A	332	GLY	5.3
2	Y	376	ALA	5.3
1	A	18	ARG	5.3
4	V	20	LEU	5.3
1	A	291	ASN	5.3
2	Y	228	ILE	5.3
1	A	696	TYR	5.2
2	Y	280	PHE	5.2
1	A	733	GLN	5.2
2	Y	326	TYR	5.1
1	A	538	TYR	5.1
1	A	288	HIS	5.1
1	A	304	VAL	5.1
2	Y	287	ILE	5.1
1	A	329	TYR	5.0
2	Y	306	TYR	5.0
2	Y	72	MET	5.0
1	A	438	ALA	5.0
1	A	225	GLY	5.0
2	Y	370	VAL	5.0
1	A	93	HIS	4.9
1	A	373	THR	4.9
1	A	242	ARG	4.9
1	A	483	ALA	4.9
4	V	108	GLY	4.9
1	A	397	PRO	4.9
2	Y	341	LYS	4.9
1	A	119	LEU	4.8
1	A	816	ASP	4.8
1	A	548	ARG	4.8
1	A	806	MET	4.8
1	A	320	THR	4.8
2	Y	15	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	717	LEU	4.8
1	A	221	LEU	4.7
1	A	545	LEU	4.7
2	Y	411	GLU	4.7
1	A	516	ARG	4.7
2	Y	237	ALA	4.7
2	Y	379	ALA	4.7
1	A	97	ILE	4.7
4	V	85	LEU	4.7
2	Y	410	LEU	4.7
2	Y	404	ILE	4.6
1	A	611	TYR	4.6
4	V	12	VAL	4.6
1	A	444	LEU	4.6
2	Y	403	LEU	4.6
1	A	436	THR	4.6
2	Y	138	GLY	4.6
3	E	21	PRO	4.6
2	Y	413	MET	4.6
1	A	19	TYR	4.5
1	A	305	ASP	4.5
1	A	707	GLN	4.5
1	A	360	TYR	4.5
1	A	525	ARG	4.5
1	A	345	ILE	4.5
3	E	8	PHE	4.5
1	A	52	LEU	4.5
3	E	29	TYR	4.5
1	A	614	ARG	4.5
2	Y	374	PHE	4.4
1	A	385	TYR	4.4
2	Y	373	LEU	4.4
1	A	175	SER	4.4
1	A	626	ILE	4.4
2	Y	407	GLY	4.3
2	Y	346	TYR	4.3
1	A	201	LEU	4.3
2	Y	286	THR	4.3
3	E	20	TRP	4.3
1	A	716	VAL	4.3
1	A	539	LEU	4.3
1	A	387	MET	4.3

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Mol	Chain	Res	Type	RSRZ
4	V	29	PHE	4.3
2	Y	328	PHE	4.2
1	A	214	ILE	4.2
1	A	400	ARG	4.2
1	A	331	GLU	4.2
1	A	215	ASP	4.2
1	A	377	GLU	4.2
2	Y	75	MET	4.2
2	Y	369	LEU	4.2
1	A	555	MET	4.2
1	A	482	ILE	4.2
2	Y	408	VAL	4.2
1	A	272	ALA	4.2
1	A	231	THR	4.1
1	A	61	LEU	4.1
1	A	731	MET	4.1
1	A	734	LEU	4.1
2	Y	42	ASP	4.1
1	A	509	GLY	4.1
1	A	353	ALA	4.1
1	A	558	LEU	4.1
2	Y	229	VAL	4.1
1	A	711	PHE	4.0
1	A	459	LEU	4.0
1	A	439	VAL	4.0
2	Y	46	LEU	4.0
1	A	458	VAL	4.0
2	Y	377	PHE	3.9
1	A	721	ASP	3.9
2	Y	322	PHE	3.9
1	A	62	LEU	3.9
3	E	31	ALA	3.9
2	Y	67	PHE	3.9
2	Y	187	ILE	3.8
1	A	537	PHE	3.8
3	E	5	THR	3.8
1	A	736	GLN	3.8
1	A	534	ILE	3.8
1	A	48	PHE	3.8
1	A	261	LEU	3.8
2	Y	244	GLN	3.8
2	Y	79	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLU	3.8
1	A	349	SER	3.8
2	Y	160	THR	3.7
1	A	381	PHE	3.7
1	A	825	ALA	3.7
4	V	82	MET	3.7
1	A	289	HIS	3.7
1	A	311	GLY	3.7
1	A	333	LEU	3.7
1	A	606	GLN	3.7
2	Y	163	LEU	3.7
2	Y	290	PHE	3.7
1	A	352	LEU	3.7
1	A	503	GLY	3.7
1	A	452	LYS	3.7
2	Y	232	ILE	3.6
2	Y	231	VAL	3.6
1	A	728	ILE	3.6
1	A	219	THR	3.5
1	A	269	ALA	3.5
1	A	25	ASP	3.5
4	V	34	MET	3.5
1	A	220	PRO	3.5
2	Y	344	GLY	3.5
1	A	547	ARG	3.5
2	Y	14	ILE	3.5
1	A	550	GLY	3.4
1	A	753	ILE	3.4
1	A	408	TYR	3.4
1	A	418	VAL	3.4
1	A	567	THR	3.4
1	A	445	ILE	3.4
1	A	531	ASP	3.4
1	A	710	GLU	3.4
1	A	134	ALA	3.4
1	A	362	ARG	3.4
1	A	789	PRO	3.4
1	A	715	ILE	3.4
1	A	460	ASN	3.4
1	A	804	PHE	3.4
1	A	388	GLN	3.3
3	E	15	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	3.3
1	A	485	ASN	3.3
2	Y	412	THR	3.3
1	A	766	ALA	3.3
1	A	318	SER	3.3
2	Y	162	PHE	3.3
1	A	250	TYR	3.3
1	A	16	LEU	3.3
2	Y	140	LEU	3.3
2	Y	186	GLY	3.3
2	Y	414	LYS	3.3
1	A	15	THR	3.3
2	Y	43	VAL	3.3
2	Y	136	ALA	3.2
1	A	205	VAL	3.2
2	Y	77	TYR	3.2
1	A	384	ILE	3.2
1	A	685	LEU	3.2
1	A	315	ILE	3.2
1	A	727	HIS	3.2
1	A	51	ARG	3.2
2	Y	78	ILE	3.2
1	A	530	GLY	3.2
1	A	448	LEU	3.2
1	A	285	ALA	3.2
1	A	433	LEU	3.2
1	A	788	GLY	3.2
2	Y	278	VAL	3.2
1	A	435	GLY	3.1
1	A	86	LEU	3.1
1	A	341	GLU	3.1
1	A	799	TYR	3.1
1	A	378	GLU	3.1
1	A	287	ASN	3.1
1	A	480	VAL	3.1
1	A	430	GLN	3.1
1	A	582	GLN	3.1
2	Y	323	THR	3.1
1	A	505	LEU	3.1
1	A	306	TYR	3.1
2	Y	409	ALA	3.1
1	A	814	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLN	3.1
2	Y	330	GLN	3.1
3	E	4	VAL	3.1
2	Y	259	SER	3.1
1	A	334	HIS	3.1
1	A	399	VAL	3.0
1	A	484	THR	3.0
1	A	559	ASP	3.0
1	A	258	ALA	3.0
1	A	259	VAL	3.0
1	A	290	ILE	3.0
1	A	762	PHE	3.0
2	Y	405	VAL	3.0
2	Y	242	PRO	3.0
1	A	386	ASN	3.0
1	A	126	VAL	3.0
1	A	390	VAL	3.0
1	A	735	ARG	3.0
1	A	59	ASP	3.0
2	Y	234	ILE	3.0
1	A	310	ASP	3.0
1	A	281	VAL	3.0
3	E	33	VAL	2.9
2	Y	315	TYR	2.9
2	Y	36	VAL	2.9
1	A	631	ILE	2.9
1	A	507	VAL	2.9
1	A	294	LEU	2.9
4	V	80	LEU	2.9
1	A	617	VAL	2.9
1	A	566	SER	2.9
1	A	184	TYR	2.9
1	A	47	GLU	2.9
1	A	810	MET	2.9
1	A	760	ALA	2.9
2	Y	364	LEU	2.9
3	E	25	GLU	2.9
1	A	730	ALA	2.9
1	A	185	LEU	2.8
2	Y	227	VAL	2.8
2	Y	239	ARG	2.8
1	A	98	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	533	GLY	2.8
1	A	271	LYS	2.8
1	A	805	ALA	2.8
2	Y	317	VAL	2.8
1	A	222	ILE	2.8
1	A	124	VAL	2.8
1	A	706	GLU	2.8
1	A	565	ASP	2.8
3	E	6	ASN	2.8
1	A	210	ASP	2.8
2	Y	318	LEU	2.8
1	A	243	THR	2.8
2	Y	137	GLY	2.8
1	A	522	LEU	2.7
2	Y	183	ILE	2.7
1	A	338	GLU	2.7
4	V	25	SER	2.7
1	A	286	LEU	2.7
1	A	409	ARG	2.7
1	A	442	SER	2.7
1	A	737	GLY	2.7
1	A	755	ILE	2.7
2	Y	82	ILE	2.7
1	A	724	TRP	2.7
1	A	419	ALA	2.7
1	A	129	VAL	2.7
4	V	47	VAL	2.7
1	A	99	GLU	2.7
1	A	602	VAL	2.7
4	V	81	GLN	2.7
1	A	207	ASP	2.6
1	A	807	PHE	2.6
1	A	763	ALA	2.6
1	A	540	SER	2.6
2	Y	372	SER	2.6
1	A	405	ASP	2.6
2	Y	422	LYS	2.6
2	Y	342	LYS	2.6
3	E	28	ASN	2.6
1	A	206	ILE	2.6
1	A	504	GLY	2.6
1	A	732	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	589	ASN	2.6
2	Y	264	LEU	2.6
2	Y	124	GLN	2.6
1	A	327	ARG	2.6
2	Y	107	ARG	2.6
1	A	506	ALA	2.5
4	V	110	GLY	2.5
1	A	312	GLN	2.5
1	A	714	VAL	2.5
1	A	491	THR	2.5
2	Y	28	PHE	2.5
1	A	635	LEU	2.5
1	A	363	MET	2.5
1	A	523	ARG	2.5
3	E	32	VAL	2.5
1	A	543	ASP	2.5
2	Y	304	PHE	2.5
2	Y	324	TYR	2.5
4	V	94	TYR	2.5
2	Y	277	ALA	2.5
1	A	116	LEU	2.5
1	A	133	LEU	2.5
1	A	216	GLU	2.4
1	A	292	GLN	2.4
1	A	58	THR	2.4
1	A	515	SER	2.4
2	Y	106	ARG	2.4
3	E	30	THR	2.4
1	A	54	LYS	2.4
1	A	257	LYS	2.4
1	A	64	GLU	2.4
2	Y	416	LEU	2.4
1	A	508	VAL	2.4
3	E	27	VAL	2.4
1	A	234	TYR	2.4
1	A	415	PHE	2.4
1	A	754	ALA	2.3
1	A	709	ARG	2.3
3	E	12	VAL	2.3
2	Y	260	THR	2.3
1	A	303	ASP	2.3
1	A	339	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	Y	320	ILE	2.3
1	A	161	LYS	2.3
1	A	328	ARG	2.3
1	A	607	ARG	2.3
1	A	96	ASN	2.3
3	E	53	GLN	2.3
1	A	518	ILE	2.3
1	A	402	ASP	2.3
1	A	368	ALA	2.3
1	A	574	VAL	2.3
1	A	223	ILE	2.2
1	A	308	VAL	2.2
1	A	343	LEU	2.2
1	A	101	LYS	2.2
4	V	116	SER	2.2
3	E	36	THR	2.2
1	A	692	ILE	2.2
1	A	454	ILE	2.2
1	A	599	TYR	2.2
1	A	208	GLU	2.2
2	Y	47	GLN	2.2
1	A	316	VAL	2.1
2	Y	380	VAL	2.1
1	A	396	ARG	2.1
2	Y	424	HIS	2.1
2	Y	429	ILE	2.1
4	V	95	CYS	2.1
2	Y	281	LEU	2.1
1	A	542	GLU	2.1
1	A	364	TYR	2.1
2	Y	190	GLY	2.1
2	Y	85	GLN	2.1
2	Y	316	VAL	2.1
1	A	618	ILE	2.0
1	A	282	LYS	2.0
1	A	517	ARG	2.0
1	A	213	LEU	2.0
2	Y	189	SER	2.0
1	A	23	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
8	TBR	A	1016	18/18	0.94	0.36	1.38	205,240,270,278	18
8	TBR	A	1010	18/18	0.92	0.26	0.59	320,422,488,488	18
8	TBR	A	1015	18/18	0.95	0.31	-0.24	150,184,202,207	18
7	ADP	A	1003	27/27	0.86	0.21	-0.37	217,228,242,264	0
8	TBR	A	1012	18/18	0.99	0.27	-0.46	262,342,436,479	0
8	TBR	A	1004	18/18	0.99	0.27	-0.51	267,292,333,345	0
8	TBR	A	1017	18/18	0.74	0.28	-0.67	239,281,307,310	18
6	BEF	A	1002	4/4	0.88	0.15	-0.75	248,258,259,292	0
8	TBR	A	1009	18/18	0.98	0.18	-0.82	315,412,481,486	18
8	TBR	Y	501	18/18	0.97	0.32	-0.89	247,285,334,358	18
8	TBR	A	1007	18/18	0.97	0.29	-0.96	204,235,270,286	18
8	TBR	A	1005	18/18	0.99	0.28	-1.03	296,311,356,389	18
8	TBR	Y	502	18/18	0.97	0.33	-1.05	214,274,323,365	18
8	TBR	A	1011	18/18	0.99	0.27	-1.19	249,291,340,349	18
8	TBR	A	1006	18/18	0.96	0.19	-1.40	261,311,368,380	18
8	TBR	A	1014	18/18	0.94	0.22	-1.54	256,294,322,323	18
8	TBR	A	1013	18/18	0.95	0.21	-1.98	212,254,282,284	18
8	TBR	Y	503	18/18	0.89	0.45	-	222,330,362,376	18
5	MG	A	1001	1/1	0.93	0.27	-	156,156,156,156	0
8	TBR	A	1018	18/18	0.87	0.42	-	249,294,327,336	18
8	TBR	A	1008	18/18	0.94	0.39	-	216,259,385,416	18

6.5 Other polymers [i](#)

There are no such residues in this entry.