



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 12:59 PM EDT

PDB ID : 1LTX
Title : Structure of Rab Escort Protein-1 in complex with Rab geranylgeranyl transferase and isoprenoid
Authors : Pylypenko, O.; Rak, A.; Reents, R.; Niculae, A.; Thoma, N.H.; Waldmann, H.; Schlichting, I.; Goody, R.S.; Alexandrov, K.
Deposited on : 2002-05-21
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

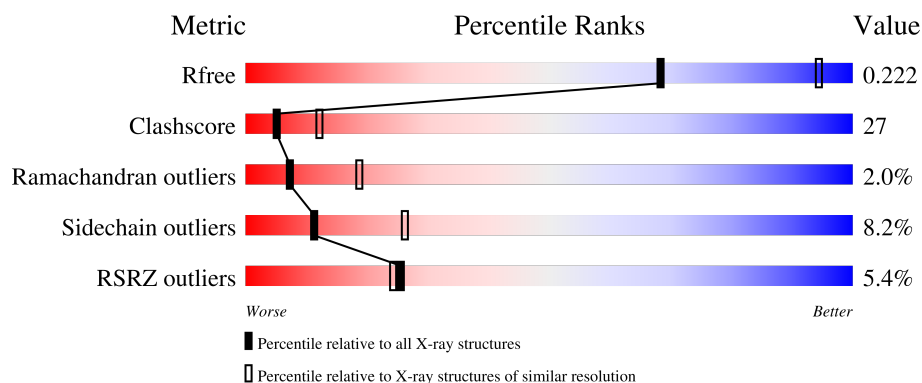
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	567	<div> <div>6%</div> <div>47%</div> <div>42%</div> <div>6%</div> <div>5%</div> </div>
2	B	331	<div> <div>3%</div> <div>48%</div> <div>42%</div> <div>5%</div> <div>.</div> </div>
3	R	650	<div> <div>4%</div> <div>44%</div> <div>29%</div> <div>.</div> <div>24%</div> </div>
4	P	4	<div> <div>75%</div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10874 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 RAB GERANYLGERANYLTRANSFERASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4291	2709	755	799	28			

- Molecule 2 is a protein called RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	318	Total	C	N	O	S	0	0	0
			2477	1582	411	464	20			

- Molecule 3 is a protein called Rab Escort Protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	494	Total	C	N	O	S	0	0	0
			3944	2494	663	758	29			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	231	LYS	GLN	engineered mutation	UNP P37727
R	473	THR	ALA	engineered mutation	UNP P37727
R	483	ALA	GLY	engineered mutation	UNP P37727

- Molecule 4 is a protein called AAAA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	4	Total	C	N	O	0	4	0
			42	24	8	10			

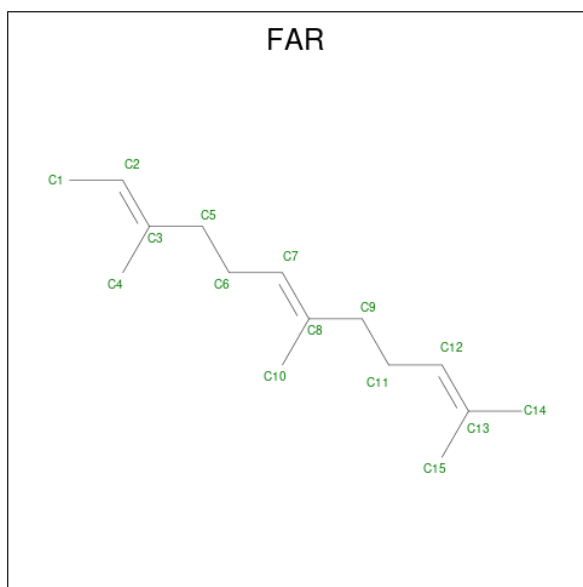
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	Cl	0	0
			1	1		

- Molecule 7 is FARNESYL (three-letter code: FAR) (formula: C₁₅H₂₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total	C	0	0
			15	15		

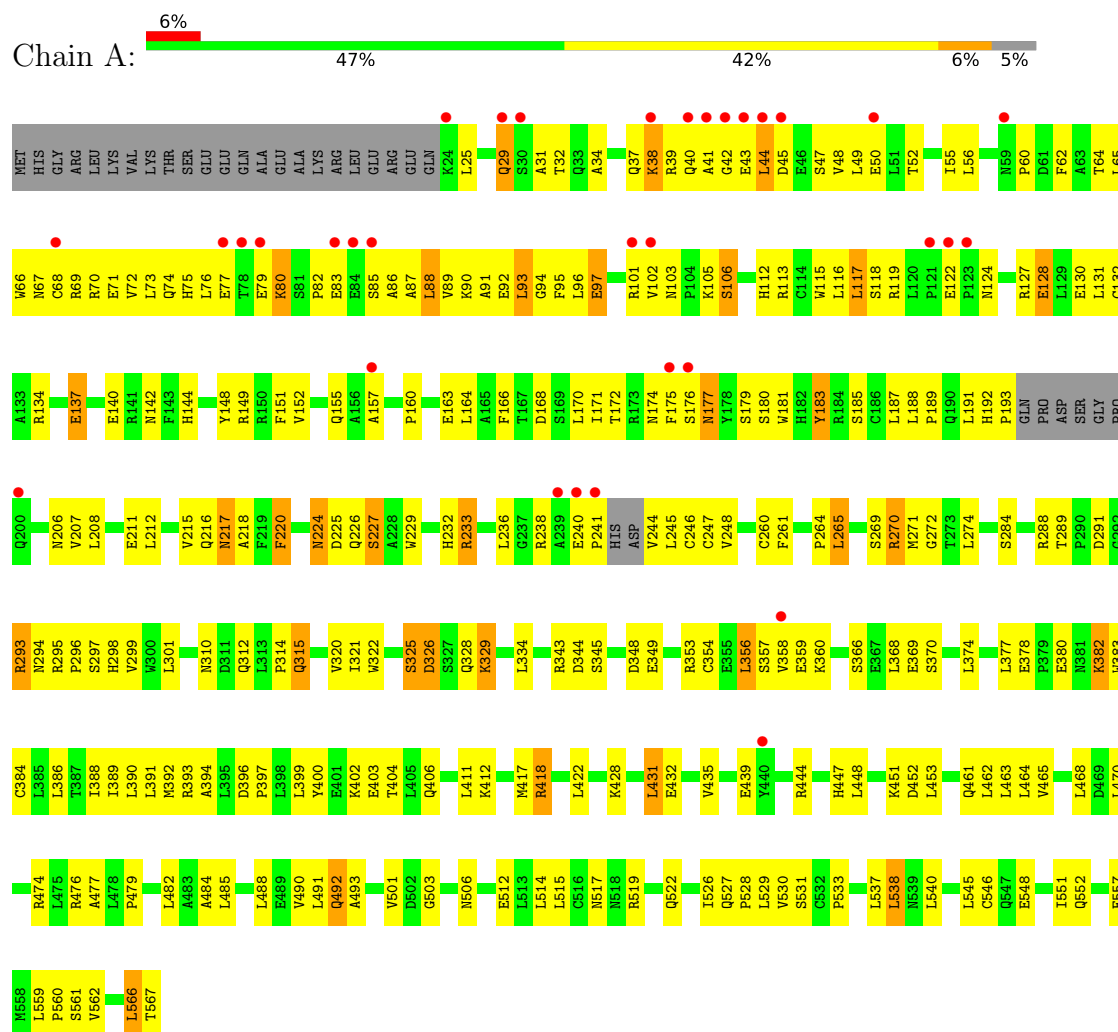
- Molecule 8 is water.

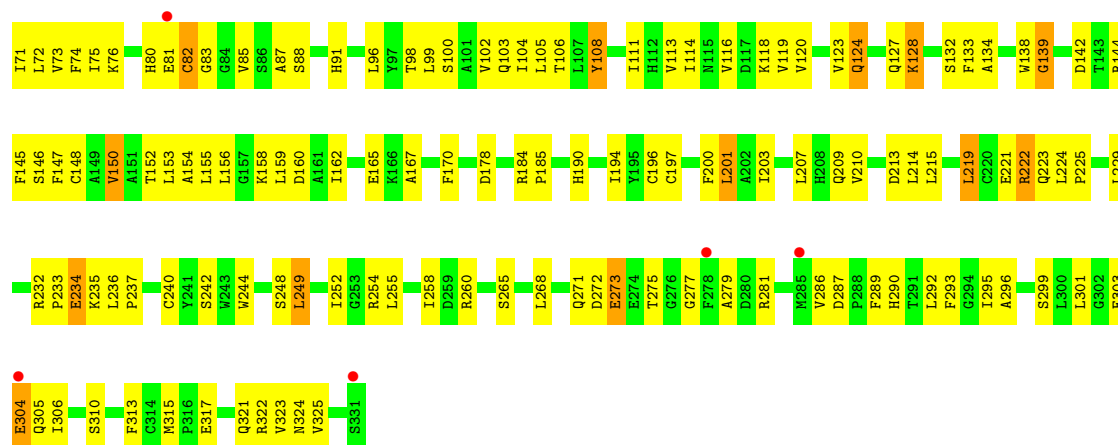
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total	O	0	0
			41	41		
8	B	20	Total	O	0	0
			20	20		
8	R	41	Total	O	0	0
			41	41		
8	P	1	Total	O	0	0
			1	1		

3 Residue-property plots

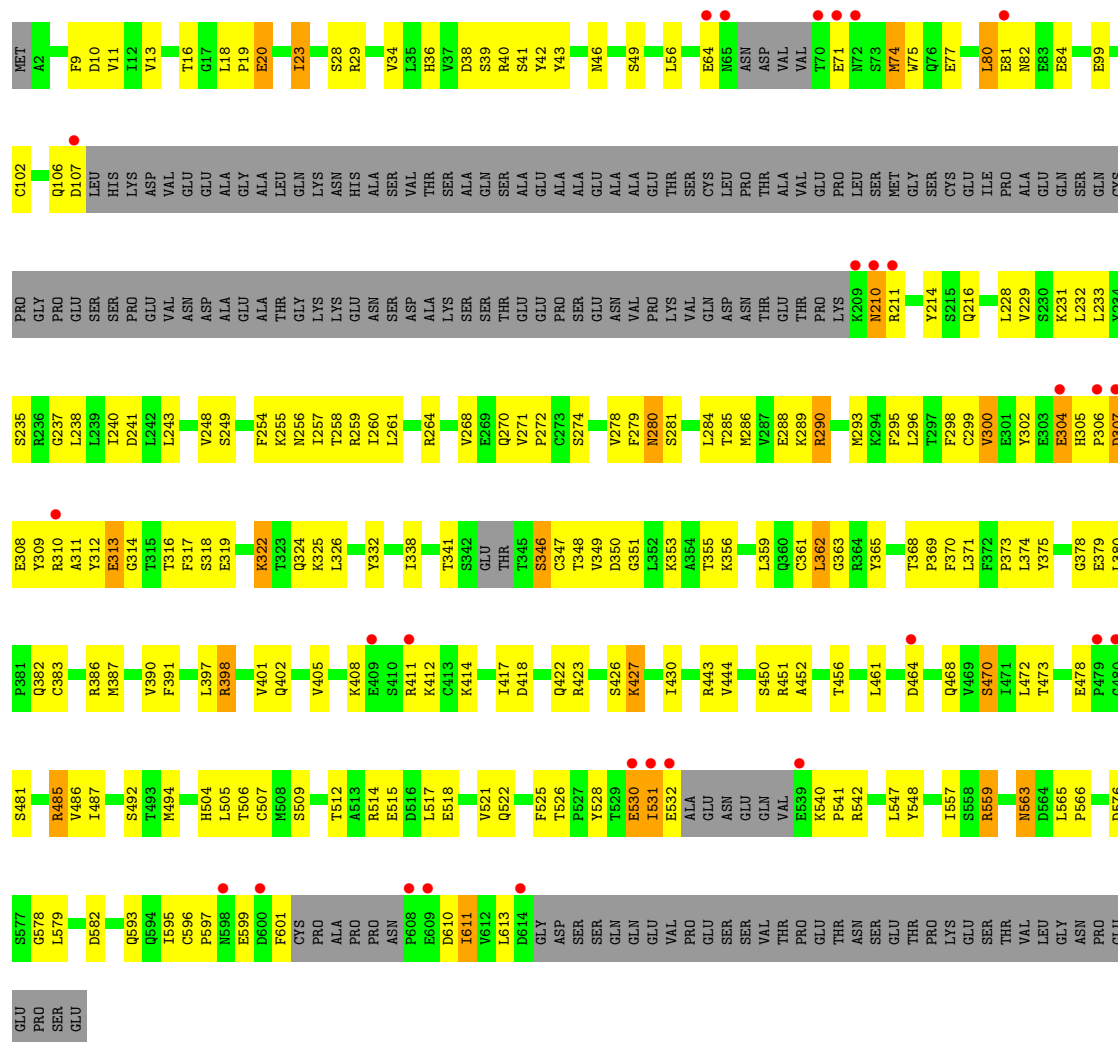
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RAB GERANYLGERANYLTRANSFERASE ALPHA SUBUNIT

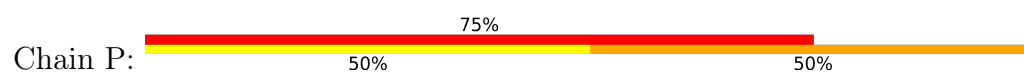




• Molecule 3: Rab Escort Protein 1



• Molecule 4: AAAA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.70Å 197.30Å 85.30Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	19.74 – 2.70 19.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.74-2.70) 94.9 (19.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.272 0.219 , 0.222	Depositor DCC
R_{free} test set	2739 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10874	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, FAR, CL

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	0.40	0/4380	0.61	1/5953 (0.0%)
2	B	0.38	0/2532	0.59	0/3428
3	R	0.44	0/4016	0.66	0/5422
4	P	0.56	0/40	0.47	0/50
All	All	0.41	0/10968	0.62	1/14853 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	PRO	N-CA-CB	5.65	110.08	103.30

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	4291	0	4252	247	0
2	B	2477	0	2434	142	0
3	R	3944	0	3891	194	0
4	P	42	0	38	9	0
5	B	1	0	0	0	0
6	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	15	0	26	3	0
8	A	41	0	0	2	0
8	B	20	0	0	0	0
8	P	1	0	0	0	0
8	R	41	0	0	2	0
All	All	10874	0	10641	575	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 27.

All (575) 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:P:12[B]:ALA:OXT	4:P:12[B]:ALA:O	1.73	1.05
1:A:71:GLU:HA	1:A:74:GLN:HE21	1.25	1.00
3:R:259:ARG:HG3	3:R:470:SER:HB3	1.44	0.99
3:R:106:GLN:HB2	3:R:214:TYR:HB3	1.46	0.97
3:R:316:THR:HG22	3:R:318:SER:H	1.27	0.96
2:B:224:LEU:HD12	2:B:237:PRO:HG3	1.47	0.95
3:R:472:LEU:HD23	3:R:473:THR:N	1.83	0.94
1:A:356:LEU:H	1:A:356:LEU:HD22	1.30	0.93
2:B:20:LEU:HD11	2:B:305:GLN:HB3	1.48	0.93
3:R:450:SER:OG	3:R:509:SER:HB3	1.70	0.92
1:A:492:GLN:HG2	1:A:514:LEU:HD12	1.52	0.92
3:R:305:HIS:HB3	3:R:308:GLU:HG3	1.51	0.92
3:R:478:GLU:HB2	3:R:481:SER:HB2	1.55	0.87
1:A:160:PRO:HB2	1:A:191:LEU:HD21	1.53	0.87
3:R:559:ARG:HH21	3:R:565:LEU:HB2	1.41	0.85
3:R:368:THR:HG23	3:R:369:PRO:HD2	1.57	0.85
4:P:12[A]:ALA:HA	7:P:1428:FAR:H42	1.58	0.85
1:A:163:GLU:HG2	1:A:183:TYR:OH	1.76	0.84
3:R:368:THR:HG22	3:R:370:PHE:H	1.39	0.84
1:A:452:ASP:OD1	1:A:474:ARG:HD3	1.80	0.82
2:B:43:GLU:HA	2:B:46:ARG:HG2	1.60	0.81
3:R:373:PRO:HG2	3:R:380:LEU:HD21	1.64	0.79
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.46	0.79
1:A:321:ILE:HG12	1:A:328:GLN:HG2	1.63	0.79
2:B:224:LEU:HD12	2:B:237:PRO:CG	2.13	0.78
2:B:100:SER:O	2:B:104:ILE:HG13	1.82	0.78
3:R:349:VAL:O	3:R:353:LYS:HG3	1.83	0.78
2:B:232:ARG:NH2	2:B:235:LYS:HZ1	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HG21	2:B:158:LYS:HG2	1.65	0.78
1:A:299:VAL:HG21	1:A:484:ALA:HA	1.66	0.78
2:B:150:VAL:HG22	2:B:159:LEU:HD11	1.65	0.77
3:R:210:ASN:N	3:R:210:ASN:HD22	1.82	0.77
3:R:596:CYS:HB3	3:R:599:GLU:HG3	1.67	0.77
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.01	0.75
3:R:305:HIS:HB3	3:R:308:GLU:CG	2.17	0.75
2:B:194:ILE:HD13	2:B:215:LEU:HD11	1.68	0.75
2:B:71:ILE:O	2:B:75:ILE:HG12	1.85	0.75
1:A:44:LEU:HD22	1:A:75:HIS:CD2	2.22	0.74
3:R:559:ARG:NH2	3:R:565:LEU:HB2	2.02	0.74
1:A:212:LEU:O	1:A:215:VAL:HG12	1.87	0.73
1:A:101:ARG:HH12	1:A:134:ARG:HH21	1.36	0.73
1:A:418:ARG:O	1:A:422:LEU:HG	1.88	0.73
2:B:52:TRP:CZ3	4:P:12[B]:ALA:OXT	2.41	0.73
1:A:343:ARG:HH21	1:A:461:GLN:HG3	1.54	0.72
1:A:240:GLU:OE2	1:A:241:PRO:HD2	1.90	0.72
3:R:281:SER:OG	3:R:284:LEU:HD13	1.88	0.72
1:A:88:LEU:HD13	1:A:91:ALA:HB3	1.71	0.72
1:A:168:ASP:O	1:A:172:THR:HG23	1.90	0.71
3:R:368:THR:HG23	3:R:369:PRO:CD	2.19	0.71
3:R:84:GLU:OE1	3:R:408:LYS:HD2	1.91	0.71
3:R:258:THR:OG1	3:R:468:GLN:HB2	1.90	0.70
1:A:382:LYS:HE2	1:A:383:TRP:CE2	2.26	0.70
3:R:231:LYS:HE2	3:R:578:GLY:O	1.90	0.70
1:A:96:LEU:HD13	1:A:113:ARG:HB2	1.71	0.70
1:A:217:ASN:HD22	1:A:218:ALA:N	1.90	0.70
1:A:171:ILE:HA	1:A:177:ASN:ND2	2.06	0.69
1:A:131:LEU:O	1:A:131:LEU:HD23	1.93	0.69
2:B:150:VAL:HG13	2:B:203:ILE:HG21	1.75	0.68
1:A:93:LEU:H	1:A:93:LEU:HD12	1.59	0.68
3:R:412:LYS:HA	3:R:566:PRO:HB3	1.76	0.68
1:A:44:LEU:HD13	1:A:75:HIS:CE1	2.28	0.68
3:R:443:ARG:HD3	3:R:563:ASN:OD1	1.94	0.67
1:A:261:PHE:CD1	1:A:265:LEU:HD11	2.29	0.67
2:B:232:ARG:NE	2:B:235:LYS:HZ2	1.93	0.67
1:A:44:LEU:HD12	1:A:44:LEU:H	1.60	0.67
1:A:527:GLN:HB3	1:A:528:PRO:HD3	1.77	0.67
2:B:248:SER:O	2:B:252:ILE:HG12	1.95	0.66
3:R:559:ARG:NH2	3:R:565:LEU:CB	2.58	0.66
2:B:222:ARG:HA	2:B:222:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HA	1:A:72:VAL:HG12	1.78	0.66
3:R:373:PRO:CG	3:R:380:LEU:HD21	2.25	0.66
3:R:313:GLU:HG3	3:R:349:VAL:CG1	2.25	0.66
3:R:347:CYS:SG	3:R:349:VAL:HG22	2.36	0.66
1:A:71:GLU:O	1:A:74:GLN:HG2	1.96	0.66
3:R:304:GLU:HB3	3:R:305:HIS:HD2	1.61	0.66
3:R:49:SER:HB2	3:R:378:GLY:HA3	1.79	0.65
3:R:82:ASN:O	3:R:408:LYS:HB2	1.96	0.65
2:B:219:LEU:HD23	2:B:249:LEU:HD13	1.78	0.65
3:R:512:THR:OG1	3:R:515:GLU:HG3	1.97	0.65
2:B:8:VAL:HG22	2:B:9:THR:N	2.12	0.64
1:A:151:PHE:O	1:A:155:GLN:HG2	1.97	0.64
1:A:183:TYR:CE1	1:A:187:LEU:HD21	2.32	0.64
1:A:66:TRP:HE3	1:A:112:HIS:ND1	1.95	0.64
1:A:166:PHE:O	1:A:170:LEU:HD23	1.96	0.64
2:B:52:TRP:HZ3	4:P:12[B]:ALA:OXT	1.80	0.64
1:A:128:GLU:HB3	1:A:152:VAL:HG11	1.79	0.64
2:B:83:GLY:HA2	2:B:118:LYS:HB3	1.78	0.64
3:R:559:ARG:HH21	3:R:565:LEU:CB	2.11	0.64
1:A:530:VAL:HG22	1:A:530:VAL:O	1.97	0.64
3:R:9:PHE:O	3:R:426:SER:HA	1.97	0.64
3:R:285:THR:OG1	3:R:288:GLU:HG3	1.98	0.64
3:R:259:ARG:NH1	3:R:461:LEU:HD23	2.12	0.63
1:A:402:LYS:O	1:A:406:GLN:HG3	1.98	0.63
1:A:60:PRO:HG3	1:A:103:ASN:ND2	2.13	0.63
3:R:280:ASN:N	3:R:280:ASN:HD22	1.97	0.63
1:A:224:ASN:N	1:A:224:ASN:HD22	1.96	0.63
1:A:270:ARG:HE	2:B:165:GLU:CD	2.01	0.63
1:A:40:GLN:HE22	1:A:41:ALA:HB2	1.64	0.62
3:R:280:ASN:HD22	3:R:280:ASN:H	1.46	0.62
1:A:220:PHE:O	3:R:290:ARG:HG2	1.99	0.62
3:R:324:GLN:HB2	3:R:326:LEU:HD23	1.82	0.62
2:B:268:LEU:O	2:B:271:GLN:HG2	1.98	0.62
3:R:238:LEU:HD13	3:R:582:ASP:OD2	1.99	0.62
2:B:20:LEU:HD11	2:B:305:GLN:CB	2.27	0.61
2:B:279:ALA:HB2	2:B:286:VAL:HG12	1.83	0.61
1:A:233:ARG:HD2	8:A:584:HOH:O	1.99	0.61
1:A:97:GLU:HB3	1:A:101:ARG:NH1	2.15	0.60
1:A:274:LEU:HD22	1:A:320:VAL:CG1	2.30	0.60
1:A:557:GLU:O	1:A:560:PRO:HD3	2.02	0.60
1:A:172:THR:HG22	3:R:279:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CYS:O	1:A:388:ILE:HG13	2.01	0.60
1:A:97:GLU:O	1:A:101:ARG:HD3	2.00	0.60
1:A:55:ILE:HD12	1:A:55:ILE:H	1.67	0.60
1:A:174:ASN:HB2	1:A:177:ASN:HD22	1.67	0.60
3:R:526:THR:HG23	3:R:540:LYS:HE3	1.83	0.60
1:A:102:VAL:HG13	1:A:103:ASN:ND2	2.17	0.60
3:R:506:THR:HG22	3:R:507:CYS:N	2.17	0.60
1:A:29:GLN:O	1:A:32:THR:HB	2.02	0.60
3:R:313:GLU:HG3	3:R:349:VAL:HG11	1.84	0.60
1:A:418:ARG:NH2	2:B:223:GLN:O	2.35	0.59
2:B:54:LEU:HD12	2:B:66:MET:HG3	1.84	0.59
1:A:270:ARG:NH1	1:A:270:ARG:HB2	2.17	0.59
1:A:289:THR:HG23	1:A:294:ASN:HA	1.83	0.59
3:R:304:GLU:HB3	3:R:305:HIS:CD2	2.37	0.59
1:A:451:LYS:HB2	1:A:453:LEU:HG	1.84	0.59
1:A:71:GLU:HA	1:A:74:GLN:NE2	2.08	0.59
1:A:75:HIS:C	1:A:76:LEU:HD12	2.22	0.59
2:B:119:VAL:O	2:B:123:VAL:HG23	2.03	0.59
1:A:66:TRP:HE3	1:A:112:HIS:HD1	1.44	0.59
3:R:237:GLY:H	3:R:240:ILE:CG2	2.15	0.59
3:R:316:THR:HG22	3:R:318:SER:N	2.10	0.59
1:A:289:THR:CG2	1:A:294:ASN:HA	2.33	0.59
3:R:40:ARG:HG2	3:R:42:TYR:CZ	2.38	0.58
3:R:237:GLY:H	3:R:240:ILE:HG22	1.67	0.58
2:B:102:VAL:HG21	2:B:152:THR:HG23	1.85	0.58
3:R:351:GLY:O	3:R:355:THR:HG23	2.03	0.58
2:B:83:GLY:CA	2:B:118:LYS:HB3	2.33	0.58
3:R:210:ASN:N	3:R:210:ASN:ND2	2.51	0.58
2:B:229:LEU:HD12	2:B:242:SER:HA	1.86	0.58
3:R:228:LEU:O	3:R:451:ARG:HD3	2.03	0.58
1:A:412:LYS:HE2	1:A:422:LEU:HB2	1.85	0.58
2:B:317:GLU:O	2:B:321:GLN:HG3	2.03	0.58
1:A:559:LEU:HB3	1:A:562:VAL:HG23	1.85	0.58
1:A:264:PRO:HG3	1:A:298:HIS:CE1	2.39	0.58
2:B:222:ARG:HA	2:B:222:ARG:HH11	1.69	0.58
1:A:82:PRO:HA	1:A:85:SER:OG	2.04	0.57
1:A:444:ARG:HD2	1:A:464:LEU:O	2.03	0.57
3:R:368:THR:CG2	3:R:369:PRO:CD	2.81	0.57
1:A:55:ILE:HD12	1:A:55:ILE:N	2.20	0.57
3:R:452:ALA:HB3	3:R:505:LEU:HB2	1.87	0.57
3:R:243:LEU:HB3	3:R:249:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TRP:CE3	1:A:112:HIS:ND1	2.69	0.57
3:R:579:LEU:O	3:R:579:LEU:HD23	2.04	0.57
1:A:260:CYS:HA	1:A:298:HIS:O	2.05	0.57
3:R:28:SER:HB3	3:R:391:PHE:HB2	1.87	0.56
3:R:248:VAL:CG1	3:R:383:CYS:HB3	2.35	0.56
3:R:472:LEU:HD23	3:R:473:THR:H	1.63	0.56
2:B:67:ASN:O	2:B:71:ILE:HG13	2.04	0.56
2:B:8:VAL:HG22	2:B:9:THR:H	1.70	0.56
3:R:506:THR:O	3:R:507:CYS:HB3	2.05	0.56
2:B:232:ARG:CZ	2:B:235:LYS:NZ	2.69	0.56
3:R:248:VAL:HG13	3:R:383:CYS:HB3	1.86	0.56
1:A:72:VAL:O	1:A:75:HIS:HB3	2.04	0.56
1:A:64:THR:HA	1:A:67:ASN:HD22	1.70	0.56
1:A:289:THR:H	1:A:294:ASN:ND2	2.04	0.56
3:R:579:LEU:HD23	3:R:579:LEU:C	2.26	0.56
1:A:241:PRO:HB2	1:A:244:VAL:HG21	1.88	0.56
3:R:374:LEU:O	3:R:375:TYR:HB2	2.05	0.56
1:A:72:VAL:HG23	1:A:73:LEU:N	2.21	0.55
1:A:226:GLN:HG2	1:A:383:TRP:CZ2	2.42	0.55
2:B:106:THR:HA	2:B:111:ILE:HD11	1.88	0.55
1:A:88:LEU:HD13	1:A:91:ALA:CB	2.37	0.55
3:R:295:PHE:O	3:R:298:PHE:HB3	2.06	0.55
3:R:304:GLU:C	3:R:305:HIS:HD2	2.10	0.55
2:B:128:LYS:HD2	2:B:128:LYS:N	2.21	0.55
2:B:116:VAL:O	2:B:120:VAL:HG23	2.07	0.55
2:B:240:CYS:HB3	2:B:290:HIS:CD2	2.41	0.55
1:A:44:LEU:HD22	1:A:75:HIS:CG	2.42	0.55
1:A:356:LEU:HD21	1:A:394:ALA:O	2.07	0.55
2:B:232:ARG:CZ	2:B:235:LYS:HZ1	2.19	0.55
3:R:80:LEU:HD13	3:R:81:GLU:H	1.72	0.55
3:R:304:GLU:C	3:R:306:PRO:HD3	2.26	0.55
1:A:160:PRO:HB2	1:A:191:LEU:CD2	2.33	0.55
2:B:303:GLU:HG2	2:B:306:ILE:CD1	2.37	0.55
1:A:310:ASN:OD1	1:A:312:GLN:HG2	2.06	0.55
1:A:88:LEU:O	1:A:91:ALA:HB3	2.07	0.55
3:R:102:CYS:SG	3:R:107:ASP:HB3	2.47	0.55
2:B:295:ILE:HG23	2:B:306:ILE:HG12	1.89	0.55
1:A:137:GLU:OE1	1:A:170:LEU:HD11	2.06	0.54
3:R:312:TYR:C	3:R:314:GLY:H	2.10	0.54
1:A:369:GLU:HG3	1:A:370:SER:N	2.23	0.54
2:B:134:ALA:HB1	2:B:139:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:HD11	2:B:162:ILE:HG23	1.89	0.54
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.72	0.54
1:A:127:ARG:HA	1:A:130:GLU:OE2	2.07	0.54
1:A:345:SER:O	1:A:349:GLU:HG2	2.07	0.54
2:B:88:SER:HB3	2:B:91:HIS:CD2	2.42	0.54
1:A:225:ASP:OD2	1:A:227:SER:HB2	2.07	0.54
2:B:68:LYS:HG2	2:B:72:LEU:HD13	1.88	0.54
1:A:315:GLN:HB3	1:A:334:LEU:HD23	1.90	0.54
1:A:220:PHE:CD2	3:R:286:MET:HG3	2.43	0.54
1:A:37:GLN:HA	1:A:37:GLN:NE2	2.23	0.54
2:B:213:ASP:OD2	2:B:254:ARG:NH1	2.40	0.54
3:R:317:PHE:CD2	3:R:351:GLY:HA3	2.43	0.54
1:A:357:SER:O	1:A:359:GLU:N	2.41	0.53
1:A:366:SER:O	1:A:369:GLU:HG2	2.08	0.53
3:R:338:ILE:N	3:R:338:ILE:HD12	2.23	0.53
3:R:368:THR:CG2	3:R:369:PRO:N	2.70	0.53
1:A:389:ILE:HG23	1:A:404:THR:HG23	1.90	0.53
1:A:89:VAL:HG12	1:A:90:LYS:N	2.22	0.53
2:B:111:ILE:HG22	2:B:111:ILE:O	2.08	0.53
3:R:368:THR:HG22	3:R:369:PRO:N	2.23	0.53
1:A:38:LYS:NZ	1:A:38:LYS:HB3	2.24	0.53
1:A:356:LEU:H	1:A:356:LEU:CD2	2.09	0.53
2:B:303:GLU:HG2	2:B:306:ILE:HD13	1.91	0.53
2:B:96:LEU:HD23	2:B:148:CYS:SG	2.49	0.53
2:B:159:LEU:O	2:B:159:LEU:HG	2.09	0.53
3:R:478:GLU:H	3:R:478:GLU:CD	2.11	0.53
1:A:80:LYS:CD	1:A:80:LYS:H	2.22	0.53
1:A:140:GLU:CD	1:A:140:GLU:H	2.12	0.53
1:A:506:ASN:H	1:A:531:SER:HB2	1.74	0.53
1:A:248:VAL:HG21	1:A:329:LYS:HB3	1.91	0.52
2:B:304:GLU:CD	2:B:304:GLU:H	2.12	0.52
1:A:131:LEU:HA	1:A:134:ARG:NH1	2.25	0.52
1:A:545:LEU:O	1:A:548:GLU:HG3	2.10	0.52
2:B:43:GLU:HA	2:B:46:ARG:CG	2.35	0.52
1:A:142:ASN:OD1	1:A:144:HIS:HB2	2.10	0.52
1:A:148:TYR:O	1:A:151:PHE:HB3	2.10	0.52
3:R:379:GLU:HG2	8:R:906:HOH:O	2.09	0.52
3:R:518:GLU:O	3:R:522:GLN:HG3	2.10	0.52
1:A:392:MET:SD	1:A:400:TYR:HB3	2.49	0.52
1:A:45:ASP:OD1	1:A:47:SER:N	2.42	0.52
1:A:545:LEU:C	1:A:545:LEU:HD12	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:456:THR:HG21	3:R:525:PHE:CE2	2.45	0.52
1:A:67:ASN:OD1	2:B:138:TRP:CD1	2.63	0.52
3:R:411:ARG:HH11	3:R:411:ARG:HG2	1.75	0.52
1:A:80:LYS:H	1:A:80:LYS:HD3	1.74	0.51
3:R:260:ILE:N	3:R:260:ILE:HD12	2.25	0.51
3:R:274:SER:O	3:R:278:VAL:HG23	2.10	0.51
1:A:77:GLU:HB2	1:A:119:ARG:HH12	1.75	0.51
2:B:43:GLU:OE2	2:B:46:ARG:HG3	2.11	0.51
3:R:405:VAL:O	3:R:414:LYS:HG2	2.11	0.51
3:R:485:ARG:O	3:R:485:ARG:HG3	2.10	0.51
1:A:87:ALA:O	1:A:90:LYS:HG2	2.10	0.51
1:A:174:ASN:HB2	1:A:177:ASN:ND2	2.25	0.51
1:A:176:SER:HA	1:A:225:ASP:OD1	2.10	0.51
1:A:70:ARG:HG3	1:A:115:TRP:CZ3	2.46	0.51
1:A:444:ARG:O	1:A:465:VAL:HG13	2.10	0.51
3:R:295:PHE:CE1	3:R:299:CYS:SG	3.04	0.51
3:R:237:GLY:O	3:R:240:ILE:HG22	2.10	0.51
3:R:39:SER:O	3:R:398:ARG:HA	2.11	0.51
3:R:84:GLU:HG3	3:R:408:LYS:CD	2.41	0.51
3:R:307:ASP:HA	3:R:310:ARG:HG2	1.92	0.51
2:B:114:ILE:HD12	2:B:114:ILE:O	2.11	0.51
3:R:485:ARG:HG2	3:R:485:ARG:HH11	1.76	0.51
1:A:52:THR:OG1	1:A:69:ARG:NH1	2.43	0.51
1:A:241:PRO:O	1:A:244:VAL:HG23	2.11	0.51
3:R:386:ARG:O	3:R:390:VAL:HG23	2.11	0.51
1:A:52:THR:O	1:A:56:LEU:HB2	2.11	0.50
1:A:233:ARG:HD3	1:A:390:LEU:HD13	1.92	0.50
2:B:80:HIS:O	2:B:82:CYS:N	2.43	0.50
3:R:341:THR:HB	3:R:346:SER:HB3	1.93	0.50
2:B:197:CYS:O	2:B:201:LEU:HD22	2.11	0.50
1:A:77:GLU:OE2	1:A:85:SER:HB2	2.11	0.50
1:A:40:GLN:HE22	1:A:41:ALA:CB	2.25	0.50
3:R:46:ASN:O	3:R:229:VAL:HG23	2.10	0.50
3:R:74:MET:SD	3:R:75:TRP:N	2.84	0.50
3:R:13:VAL:HB	3:R:36:HIS:CD2	2.46	0.50
1:A:232:HIS:CE1	1:A:236:LEU:HD21	2.47	0.50
1:A:447:HIS:O	1:A:448:LEU:HD23	2.11	0.50
1:A:322:TRP:O	1:A:326:ASP:HA	2.12	0.50
1:A:92:GLU:O	1:A:95:PHE:N	2.45	0.50
3:R:272:PRO:HG2	3:R:284:LEU:HD11	1.94	0.50
2:B:234:GLU:O	2:B:235:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:261:LEU:HD21	3:R:461:LEU:HD22	1.94	0.49
3:R:506:THR:HG22	3:R:507:CYS:H	1.76	0.49
1:A:559:LEU:HB3	1:A:562:VAL:CG2	2.41	0.49
1:A:93:LEU:H	1:A:93:LEU:CD1	2.24	0.49
2:B:197:CYS:O	2:B:201:LEU:HB2	2.12	0.49
1:A:131:LEU:O	1:A:134:ARG:HB3	2.12	0.49
1:A:232:HIS:O	1:A:236:LEU:CD2	2.61	0.49
3:R:525:PHE:HD2	3:R:541:PRO:HB2	1.77	0.49
3:R:305:HIS:CD2	3:R:305:HIS:N	2.78	0.49
3:R:305:HIS:N	3:R:306:PRO:HD3	2.27	0.49
2:B:178:ASP:O	2:B:214:LEU:HD22	2.12	0.49
1:A:171:ILE:HG13	1:A:180:SER:OG	2.13	0.49
1:A:73:LEU:HD12	1:A:73:LEU:C	2.33	0.48
2:B:232:ARG:NE	2:B:235:LYS:NZ	2.60	0.48
1:A:117:LEU:HG	1:A:128:GLU:OE1	2.13	0.48
3:R:255:LYS:HZ2	3:R:492:SER:HB2	1.78	0.48
1:A:247:CYS:SG	1:A:463:LEU:HD22	2.53	0.48
1:A:531:SER:O	1:A:533:PRO:HD3	2.13	0.48
2:B:144:ARG:HD2	7:P:1428:FAR:H62	1.94	0.48
3:R:526:THR:CG2	3:R:540:LYS:HE3	2.44	0.48
2:B:201:LEU:HB3	2:B:207:LEU:HD23	1.96	0.48
2:B:272:ASP:HB2	2:B:286:VAL:HG11	1.94	0.48
3:R:261:LEU:CD2	3:R:461:LEU:HD22	2.43	0.48
1:A:31:ALA:O	1:A:34:ALA:HB3	2.13	0.48
1:A:310:ASN:HD21	1:A:312:GLN:NE2	2.12	0.48
1:A:476:ARG:O	1:A:477:ALA:HB2	2.13	0.48
2:B:72:LEU:HG	2:B:113:VAL:HG21	1.96	0.48
2:B:223:GLN:HB2	2:B:229:LEU:CD2	2.43	0.48
3:R:289:LYS:O	3:R:293:MET:HB2	2.14	0.48
1:A:261:PHE:CE1	1:A:265:LEU:HD11	2.48	0.48
2:B:43:GLU:CD	2:B:46:ARG:HG3	2.34	0.48
2:B:45:LEU:HA	2:B:87:ALA:HB1	1.96	0.48
3:R:530:GLU:C	3:R:532:GLU:H	2.15	0.48
1:A:93:LEU:HD12	1:A:93:LEU:N	2.26	0.48
2:B:190:HIS:NE2	4:P:12[A]:ALA:OXT	2.46	0.48
3:R:595:ILE:O	3:R:597:PRO:HD3	2.13	0.48
1:A:400:TYR:HA	1:A:403:GLU:OE1	2.13	0.48
2:B:236:LEU:N	2:B:236:LEU:HD12	2.28	0.48
1:A:345:SER:HB3	1:A:348:ASP:HB2	1.95	0.48
3:R:485:ARG:HG2	3:R:485:ARG:NH1	2.29	0.48
1:A:37:GLN:O	1:A:40:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:TRP:CH2	2:B:289:PHE:HZ	2.32	0.47
3:R:82:ASN:C	3:R:408:LYS:HB2	2.34	0.47
3:R:107:ASP:HB2	3:R:214:TYR:CD2	2.48	0.47
1:A:368:LEU:HA	1:A:391:LEU:HD13	1.95	0.47
1:A:382:LYS:HE2	1:A:383:TRP:CZ2	2.48	0.47
3:R:451:ARG:NH2	3:R:504:HIS:HB3	2.28	0.47
1:A:48:VAL:O	1:A:52:THR:HG23	2.15	0.47
1:A:291:ASP:CG	1:A:293:ARG:HG3	2.33	0.47
1:A:322:TRP:CD1	1:A:325:SER:HB3	2.49	0.47
1:A:382:LYS:HE2	1:A:383:TRP:CD2	2.50	0.47
2:B:120:VAL:O	2:B:124:GLN:HG2	2.15	0.47
2:B:229:LEU:O	2:B:237:PRO:HA	2.15	0.47
2:B:232:ARG:NH2	2:B:235:LYS:NZ	2.58	0.47
2:B:53:GLY:O	2:B:56:VAL:HG12	2.14	0.47
2:B:69:GLU:O	2:B:73:VAL:HG23	2.14	0.47
2:B:132:SER:HB3	2:B:170:PHE:CE1	2.49	0.47
3:R:240:ILE:HG23	3:R:241:ASP:N	2.28	0.47
3:R:316:THR:HB	3:R:319:GLU:HB2	1.96	0.47
1:A:192:HIS:CG	1:A:207:VAL:HG21	2.50	0.47
1:A:380:GLU:HB3	8:A:601:HOH:O	2.14	0.47
1:A:435:VAL:O	1:A:439:GLU:HG3	2.15	0.47
3:R:310:ARG:HD2	3:R:311:ALA:N	2.30	0.47
3:R:322:LYS:HB2	3:R:322:LYS:NZ	2.30	0.47
3:R:512:THR:HG23	3:R:515:GLU:OE2	2.15	0.47
1:A:92:GLU:O	1:A:94:GLY:N	2.48	0.47
1:A:163:GLU:HG2	1:A:183:TYR:CZ	2.50	0.47
2:B:85:VAL:HB	2:B:98:THR:HA	1.96	0.47
2:B:132:SER:HB3	2:B:170:PHE:CZ	2.50	0.47
1:A:538:LEU:HD22	1:A:540:LEU:HG	1.95	0.47
1:A:31:ALA:CB	1:A:55:ILE:HD11	2.45	0.47
2:B:106:THR:HG21	2:B:155:LEU:HD22	1.95	0.47
3:R:405:VAL:HG11	3:R:423:ARG:HH22	1.79	0.47
1:A:291:ASP:O	1:A:293:ARG:HG2	2.15	0.46
2:B:156:LEU:O	2:B:158:LYS:HD3	2.14	0.46
3:R:84:GLU:HG3	3:R:408:LYS:HD3	1.97	0.46
1:A:40:GLN:NE2	1:A:41:ALA:N	2.63	0.46
2:B:11:LYS:NZ	2:B:265:SER:HB3	2.30	0.46
3:R:302:TYR:CE2	3:R:356:LYS:HD3	2.51	0.46
3:R:452:ALA:HA	3:R:547:LEU:O	2.15	0.46
3:R:559:ARG:NH2	3:R:565:LEU:HB3	2.29	0.46
3:R:559:ARG:NH1	8:R:909:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:CD	1:A:80:LYS:N	2.78	0.46
1:A:431:LEU:O	1:A:435:VAL:HG23	2.14	0.46
1:A:529:LEU:N	1:A:529:LEU:HD12	2.30	0.46
2:B:52:TRP:HA	2:B:292:LEU:HD22	1.98	0.46
3:R:259:ARG:HB3	3:R:270:GLN:NE2	2.30	0.46
3:R:261:LEU:HD22	3:R:268:VAL:CG1	2.46	0.46
1:A:124:ASN:CG	1:A:124:ASN:O	2.54	0.46
1:A:546:CYS:SG	1:A:567:THR:OXT	2.72	0.46
3:R:382:GLN:O	3:R:386:ARG:HG3	2.15	0.46
1:A:172:THR:HG22	3:R:279:PHE:CD2	2.50	0.46
1:A:396:ASP:CG	1:A:399:LEU:HB2	2.36	0.46
2:B:153:LEU:HB3	2:B:159:LEU:HA	1.97	0.46
1:A:288:ARG:HA	1:A:294:ASN:ND2	2.30	0.46
2:B:23:HIS:ND1	2:B:277:GLY:N	2.64	0.46
3:R:444:VAL:CG1	3:R:557:ILE:HD13	2.44	0.46
1:A:75:HIS:O	1:A:79:GLU:HG3	2.15	0.46
1:A:357:SER:O	1:A:360:LYS:N	2.49	0.46
3:R:20:GLU:O	3:R:23:ILE:HG22	2.16	0.46
1:A:115:TRP:CZ2	1:A:119:ARG:HD2	2.51	0.46
1:A:493:ALA:HB3	1:A:515:LEU:HD23	1.98	0.46
2:B:142:ASP:HB3	2:B:145:PHE:CD1	2.50	0.46
3:R:233:LEU:HD22	3:R:254:PHE:CE1	2.50	0.46
3:R:595:ILE:C	3:R:597:PRO:HD3	2.36	0.46
1:A:49:LEU:HD12	1:A:72:VAL:HG23	1.98	0.45
2:B:127:GLN:NE2	2:B:167:ALA:HB2	2.31	0.45
3:R:232:LEU:HD22	3:R:257:ILE:HD11	1.98	0.45
3:R:309:TYR:O	3:R:312:TYR:N	2.42	0.45
3:R:324:GLN:HE21	3:R:324:GLN:N	2.14	0.45
1:A:37:GLN:NE2	1:A:40:GLN:HG2	2.31	0.45
1:A:44:LEU:HD12	1:A:44:LEU:N	2.29	0.45
1:A:64:THR:O	1:A:67:ASN:HB2	2.16	0.45
1:A:92:GLU:C	1:A:94:GLY:N	2.69	0.45
3:R:18:LEU:HB3	3:R:19:PRO:CD	2.45	0.45
3:R:74:MET:HE1	3:R:402:GLN:HG3	1.96	0.45
1:A:295:ARG:HB3	1:A:296:PRO:CD	2.46	0.45
3:R:302:TYR:CD2	3:R:356:LYS:HD3	2.52	0.45
3:R:405:VAL:HG11	3:R:423:ARG:NH2	2.32	0.45
1:A:417:MET:CE	2:B:225:PRO:HA	2.47	0.45
1:A:527:GLN:O	1:A:530:VAL:HG12	2.15	0.45
3:R:300:VAL:HG13	3:R:359:LEU:HB2	1.98	0.45
1:A:31:ALA:HB3	1:A:55:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD1	1:A:293:ARG:HG3	2.17	0.45
1:A:64:THR:HG21	2:B:91:HIS:HA	1.98	0.45
1:A:66:TRP:O	1:A:70:ARG:HB2	2.15	0.45
1:A:269:SER:O	1:A:270:ARG:C	2.55	0.45
1:A:531:SER:O	1:A:533:PRO:CD	2.65	0.45
2:B:23:HIS:HE1	2:B:271:GLN:HB2	1.81	0.45
3:R:248:VAL:HG22	3:R:387:MET:HG3	1.98	0.45
3:R:325:LYS:C	3:R:326:LEU:HD22	2.37	0.45
3:R:365:TYR:HE1	3:R:610:ASP:OD2	2.00	0.45
1:A:468:LEU:HD21	1:A:470:LEU:HD11	1.99	0.45
1:A:519:ARG:HG2	1:A:519:ARG:HH11	1.82	0.45
2:B:105:LEU:CD2	2:B:114:ILE:HG13	2.46	0.45
2:B:127:GLN:HB2	2:B:133:PHE:CZ	2.52	0.45
3:R:451:ARG:HH22	3:R:504:HIS:HB3	1.82	0.45
1:A:217:ASN:HA	1:A:220:PHE:HB2	1.99	0.45
1:A:343:ARG:NH2	1:A:461:GLN:HG3	2.26	0.45
2:B:232:ARG:HB2	2:B:233:PRO:CD	2.47	0.45
3:R:547:LEU:HD12	3:R:548:TYR:N	2.32	0.45
1:A:82:PRO:O	1:A:86:ALA:HB3	2.17	0.45
2:B:150:VAL:HG13	2:B:203:ILE:CG2	2.45	0.45
2:B:260:ARG:HG3	2:B:301:LEU:HD22	1.99	0.45
1:A:105:LYS:O	1:A:106:SER:HB2	2.16	0.44
3:R:304:GLU:C	3:R:305:HIS:CD2	2.89	0.44
3:R:611:ILE:CD1	3:R:613:LEU:HD21	2.47	0.44
1:A:226:GLN:O	1:A:229:TRP:HB2	2.17	0.44
1:A:270:ARG:O	1:A:272:GLY:N	2.51	0.44
2:B:293:PHE:HA	2:B:296:ALA:HB3	2.00	0.44
2:B:74:PHE:HZ	2:B:88:SER:HA	1.82	0.44
1:A:164:LEU:HD22	1:A:191:LEU:CD1	2.48	0.44
2:B:8:VAL:CG2	2:B:9:THR:N	2.78	0.44
2:B:10:ILE:N	2:B:10:ILE:HD12	2.33	0.44
3:R:298:PHE:HE1	3:R:305:HIS:HB2	1.83	0.44
1:A:344:ASP:HB3	1:A:349:GLU:HG3	2.00	0.44
3:R:41:SER:HB3	3:R:398:ARG:HD3	2.00	0.44
3:R:373:PRO:HG2	3:R:380:LEU:CD2	2.39	0.44
3:R:478:GLU:CD	3:R:478:GLU:N	2.71	0.44
3:R:576:ASP:OD1	3:R:578:GLY:N	2.50	0.44
1:A:211:GLU:HA	1:A:211:GLU:OE1	2.18	0.44
1:A:526:ILE:HG22	1:A:526:ILE:O	2.18	0.44
2:B:232:ARG:HB2	2:B:233:PRO:HD2	1.99	0.44
1:A:76:LEU:HD23	1:A:80:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:O	1:A:220:PHE:HD2	2.00	0.44
2:B:221:GLU:OE2	2:B:221:GLU:HA	2.16	0.44
2:B:323:VAL:HG12	2:B:323:VAL:O	2.18	0.44
1:A:448:LEU:HD12	1:A:470:LEU:CD2	2.48	0.44
3:R:99:GLU:OE1	3:R:514:ARG:HD3	2.17	0.44
3:R:368:THR:CG2	3:R:369:PRO:HD2	2.35	0.44
1:A:185:SER:O	1:A:189:PRO:HG2	2.18	0.43
1:A:530:VAL:O	1:A:530:VAL:CG2	2.65	0.43
2:B:190:HIS:O	2:B:194:ILE:HG13	2.18	0.43
3:R:255:LYS:HG3	3:R:256:ASN:N	2.33	0.43
1:A:566:LEU:HD13	1:A:566:LEU:N	2.33	0.43
2:B:49:GLY:HA2	2:B:52:TRP:CE3	2.53	0.43
1:A:41:ALA:HB3	1:A:43:GLU:OE1	2.18	0.43
1:A:48:VAL:CG2	1:A:72:VAL:HG11	2.47	0.43
1:A:68:CYS:HA	1:A:71:GLU:OE2	2.18	0.43
2:B:249:LEU:HD12	2:B:254:ARG:HB2	1.99	0.43
2:B:255:LEU:HD23	2:B:255:LEU:O	2.19	0.43
3:R:528:TYR:HA	3:R:542:ARG:HH21	1.82	0.43
1:A:131:LEU:HD23	1:A:131:LEU:C	2.38	0.43
1:A:128:GLU:HG3	1:A:148:TYR:HE1	1.83	0.43
2:B:30:TYR:O	2:B:32:SER:N	2.51	0.43
3:R:387:MET:O	3:R:390:VAL:HB	2.19	0.43
1:A:74:GLN:HA	1:A:119:ARG:HH22	1.84	0.43
1:A:393:ARG:O	1:A:397:PRO:HG3	2.19	0.43
1:A:512:GLU:HG2	1:A:537:LEU:HB3	2.00	0.43
2:B:19:LEU:CD1	2:B:273:GLU:HA	2.48	0.43
2:B:184:ARG:O	2:B:185:PRO:C	2.57	0.43
3:R:305:HIS:CB	3:R:308:GLU:HG3	2.37	0.43
1:A:314:PRO:C	1:A:315:GLN:HG3	2.36	0.43
2:B:56:VAL:HG13	2:B:57:MET:N	2.34	0.43
2:B:76:LYS:HA	2:B:76:LYS:HD2	1.89	0.43
2:B:215:LEU:O	2:B:219:LEU:HB2	2.18	0.43
3:R:43:TYR:CZ	3:R:397:LEU:HD11	2.53	0.43
3:R:317:PHE:HA	3:R:348:THR:HA	1.99	0.43
1:A:155:GLN:C	1:A:157:ALA:H	2.22	0.43
1:A:417:MET:HE3	2:B:225:PRO:HA	2.01	0.43
1:A:132:CYS:C	1:A:134:ARG:N	2.71	0.43
1:A:566:LEU:HD22	1:A:566:LEU:H	1.83	0.43
2:B:8:VAL:CG2	2:B:9:THR:H	2.32	0.43
2:B:108:TYR:HD2	2:B:108:TYR:HA	1.74	0.43
1:A:377:LEU:HD23	3:R:325:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ASP:OD2	4:P:9[A]:ALA:HB3	2.19	0.43
2:B:310:SER:HA	2:B:317:GLU:OE1	2.19	0.43
2:B:313:PHE:O	2:B:315:MET:HG3	2.18	0.43
3:R:10:ASP:HA	3:R:427:LYS:HD3	2.00	0.43
3:R:264:ARG:HD3	3:R:332:TYR:CD2	2.54	0.43
3:R:401:VAL:HA	3:R:418:ASP:HA	2.01	0.43
3:R:531:ILE:O	3:R:531:ILE:HG22	2.19	0.43
3:R:611:ILE:HD11	3:R:613:LEU:HD21	2.01	0.43
1:A:40:GLN:CD	1:A:41:ALA:N	2.72	0.42
2:B:224:LEU:HD12	2:B:237:PRO:CD	2.49	0.42
1:A:288:ARG:HA	1:A:294:ASN:HD21	1.84	0.42
1:A:428:LYS:O	1:A:432:GLU:HG3	2.18	0.42
3:R:347:CYS:O	3:R:350:ASP:HB2	2.18	0.42
2:B:299:SER:HB2	2:B:306:ILE:HG21	2.00	0.42
2:B:323:VAL:O	2:B:325:VAL:HG23	2.18	0.42
3:R:280:ASN:N	3:R:280:ASN:ND2	2.65	0.42
2:B:200:PHE:CD1	2:B:200:PHE:C	2.92	0.42
1:A:48:VAL:HG21	1:A:72:VAL:HG11	2.01	0.42
2:B:147:PHE:HB2	2:B:196:CYS:HB3	2.01	0.42
2:B:154:ALA:C	2:B:156:LEU:H	2.23	0.42
3:R:232:LEU:HG	3:R:487:ILE:HD13	2.02	0.42
3:R:264:ARG:HD3	3:R:332:TYR:CE2	2.54	0.42
7:P:1428:FAR:H111	7:P:1428:FAR:H101	1.84	0.42
3:R:256:ASN:ND2	3:R:371:LEU:HD23	2.35	0.42
3:R:302:TYR:O	3:R:309:TYR:HE2	2.03	0.42
3:R:380:LEU:N	3:R:380:LEU:HD22	2.34	0.42
3:R:211:ARG:HD2	3:R:528:TYR:OH	2.19	0.42
3:R:284:LEU:HD12	3:R:284:LEU:N	2.34	0.42
3:R:417:ILE:HA	3:R:422:GLN:O	2.20	0.42
1:A:132:CYS:SG	1:A:149:ARG:HB2	2.60	0.42
2:B:184:ARG:HB2	2:B:185:PRO:CD	2.50	0.42
3:R:235:SER:HB2	3:R:361:CYS:HB3	2.02	0.42
3:R:248:VAL:HG22	3:R:387:MET:CG	2.50	0.42
3:R:295:PHE:CD2	3:R:326:LEU:HD21	2.55	0.42
1:A:245:LEU:HD23	1:A:329:LYS:HB2	2.02	0.42
1:A:551:ILE:HG23	1:A:552:GLN:N	2.35	0.42
2:B:249:LEU:HD12	2:B:249:LEU:HA	1.90	0.42
3:R:261:LEU:HD12	3:R:470:SER:HB2	2.02	0.42
1:A:40:GLN:NE2	1:A:41:ALA:HB2	2.32	0.41
1:A:25:LEU:HD12	1:A:25:LEU:C	2.40	0.41
1:A:77:GLU:HB2	1:A:119:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:284:LEU:HA	3:R:288:GLU:OE1	2.19	0.41
1:A:479:PRO:O	1:A:503:GLY:HA3	2.19	0.41
1:A:220:PHE:CG	3:R:286:MET:HG3	2.56	0.41
2:B:99:LEU:HD22	2:B:148:CYS:HA	2.01	0.41
2:B:100:SER:HA	2:B:103:GLN:NE2	2.36	0.41
3:R:362:LEU:HD23	3:R:363:GLY:H	1.84	0.41
1:A:149:ARG:CZ	1:A:163:GLU:OE1	2.68	0.41
2:B:289:PHE:CE2	4:P:10[A]:ALA:HB2	2.56	0.41
3:R:16:THR:HG23	3:R:38:ASP:HB2	2.01	0.41
3:R:259:ARG:C	3:R:260:ILE:HD12	2.41	0.41
1:A:29:GLN:NE2	1:A:29:GLN:C	2.74	0.41
1:A:37:GLN:C	1:A:39:ARG:H	2.23	0.41
1:A:132:CYS:O	1:A:134:ARG:N	2.53	0.41
2:B:272:ASP:CG	2:B:275:THR:HG1	2.22	0.41
3:R:313:GLU:HG3	3:R:349:VAL:HG12	2.01	0.41
1:A:65:LEU:C	1:A:67:ASN:N	2.71	0.41
1:A:183:TYR:HE1	1:A:187:LEU:HD21	1.82	0.41
2:B:322:ARG:C	2:B:324:ASN:H	2.23	0.41
3:R:307:ASP:CG	3:R:310:ARG:HG2	2.40	0.41
3:R:517:LEU:O	3:R:521:VAL:HG23	2.20	0.41
1:A:49:LEU:HD23	1:A:49:LEU:O	2.21	0.41
1:A:488:LEU:HD11	1:A:490:VAL:O	2.21	0.41
2:B:155:LEU:O	2:B:156:LEU:HD12	2.20	0.41
4:P:10[B]:ALA:HB1	4:P:11[B]:ALA:H	1.75	0.41
1:A:79:GLU:HB2	1:A:80:LYS:H	1.60	0.41
1:A:116:LEU:C	1:A:118:SER:H	2.23	0.41
1:A:128:GLU:HA	1:A:128:GLU:OE2	2.20	0.41
1:A:236:LEU:N	1:A:236:LEU:HD22	2.36	0.41
2:B:41:MET:H	2:B:41:MET:HG2	1.68	0.41
2:B:56:VAL:O	2:B:60:MET:HG3	2.21	0.41
2:B:142:ASP:OD1	2:B:144:ARG:HB2	2.21	0.41
3:R:229:VAL:HG12	3:R:231:LYS:HG3	2.02	0.41
3:R:296:LEU:O	3:R:300:VAL:HG22	2.21	0.41
3:R:361:CYS:HB2	3:R:369:PRO:HB3	2.03	0.41
3:R:362:LEU:HD23	3:R:363:GLY:N	2.36	0.41
1:A:66:TRP:HB3	1:A:70:ARG:NH2	2.36	0.41
2:B:184:ARG:HB2	2:B:185:PRO:HD2	2.03	0.41
3:R:478:GLU:HB2	3:R:481:SER:CB	2.40	0.41
1:A:177:ASN:O	1:A:181:TRP:HD1	2.04	0.40
1:A:274:LEU:HD22	1:A:320:VAL:HG13	2.03	0.40
2:B:9:THR:HG21	2:B:281:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:SER:HA	2:B:103:GLN:HE21	1.86	0.40
2:B:201:LEU:HD23	2:B:210:VAL:CG2	2.50	0.40
3:R:23:ILE:HG21	3:R:430:ILE:HD13	2.02	0.40
3:R:312:TYR:C	3:R:314:GLY:N	2.75	0.40
1:A:88:LEU:HA	1:A:91:ALA:CB	2.52	0.40
1:A:482:LEU:HD12	1:A:485:LEU:HD13	2.02	0.40
2:B:52:TRP:CH2	4:P:12[B]:ALA:OXT	2.73	0.40
1:A:164:LEU:HD21	1:A:188:LEU:HD21	2.03	0.40
1:A:265:LEU:HD12	1:A:265:LEU:C	2.42	0.40
2:B:158:LYS:C	2:B:160:ASP:H	2.25	0.40
1:A:79:GLU:HB2	1:A:80:LYS:HD3	2.03	0.40
3:R:316:THR:HG21	3:R:318:SER:OG	2.22	0.40
2:B:215:LEU:HG	2:B:219:LEU:HD22	2.03	0.40
3:R:271:VAL:HA	3:R:272:PRO:HD3	1.88	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	530/567 (94%)	448 (84%)	69 (13%)	13 (2%)	5	14
2	B	312/331 (94%)	267 (86%)	38 (12%)	7 (2%)	6	17
3	R	482/650 (74%)	432 (90%)	46 (10%)	4 (1%)	19	43
4	P	4/4 (100%)	0	0	4 (100%)	0	0
All	All	1328/1552 (86%)	1147 (86%)	153 (12%)	28 (2%)	7	18

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	VAL

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Mol	Chain	Res	Type
2	B	16	ASP
2	B	30	TYR
3	R	611	ILE
4	P	10[A]	ALA
4	P	10[B]	ALA
1	A	80	LYS
1	A	106	SER
1	A	270	ARG
2	B	31	GLY
2	B	81	GLU
2	B	139	GLY
3	R	563	ASN
4	P	11[A]	ALA
4	P	11[B]	ALA
1	A	271	MET
1	A	325	SER
1	A	354	CYS
2	B	82	CYS
1	A	93	LEU
1	A	517	ASN
2	B	41	MET
1	A	117	LEU
1	A	227	SER
3	R	313	GLU
3	R	531	ILE
1	A	38	LYS
1	A	42	GLY

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	477/508 (94%)	430 (90%)	47 (10%)	8	18
2	B	273/284 (96%)	254 (93%)	19 (7%)	15	35
3	R	447/581 (77%)	415 (93%)	32 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1197/1373 (87%)	1099 (92%)	98 (8%)	11	26

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	44	LEU
1	A	50	GLU
1	A	62	PHE
1	A	83	GLU
1	A	88	LEU
1	A	97	GLU
1	A	122	GLU
1	A	128	GLU
1	A	137	GLU
1	A	175	PHE
1	A	177	ASN
1	A	179	SER
1	A	183	TYR
1	A	206	ASN
1	A	208	LEU
1	A	217	ASN
1	A	220	PHE
1	A	224	ASN
1	A	233	ARG
1	A	238	ARG
1	A	246	CYS
1	A	265	LEU
1	A	284	SER
1	A	293	ARG
1	A	297	SER
1	A	301	LEU
1	A	315	GLN
1	A	326	ASP
1	A	329	LYS
1	A	353	ARG
1	A	356	LEU
1	A	374	LEU
1	A	378	GLU
1	A	382	LYS
1	A	386	LEU
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	418	ARG
1	A	431	LEU
1	A	462	LEU
1	A	491	LEU
1	A	492	GLN
1	A	501	VAL
1	A	522	GLN
1	A	538	LEU
1	A	561	SER
1	A	566	LEU
2	B	22	LYS
2	B	45	LEU
2	B	54	LEU
2	B	62	GLN
2	B	69	GLU
2	B	108	TYR
2	B	124	GLN
2	B	128	LYS
2	B	146	SER
2	B	150	VAL
2	B	201	LEU
2	B	209	GLN
2	B	219	LEU
2	B	222	ARG
2	B	234	GLU
2	B	249	LEU
2	B	258	ILE
2	B	273	GLU
2	B	304	GLU
3	R	11	VAL
3	R	20	GLU
3	R	23	ILE
3	R	29	ARG
3	R	34	VAL
3	R	56	LEU
3	R	64	GLU
3	R	71	GLU
3	R	74	MET
3	R	77	GLU
3	R	80	LEU
3	R	210	ASN
3	R	216	GLN

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Mol	Chain	Res	Type
3	R	280	ASN
3	R	290	ARG
3	R	300	VAL
3	R	304	GLU
3	R	307	ASP
3	R	322	LYS
3	R	346	SER
3	R	362	LEU
3	R	398	ARG
3	R	427	LYS
3	R	464	ASP
3	R	470	SER
3	R	485	ARG
3	R	486	VAL
3	R	494	MET
3	R	530	GLU
3	R	559	ARG
3	R	593	GLN
3	R	601	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	GLN
1	A	37	GLN
1	A	40	GLN
1	A	74	GLN
1	A	75	HIS
1	A	103	ASN
1	A	111	HIS
1	A	174	ASN
1	A	177	ASN
1	A	216	GLN
1	A	217	ASN
1	A	224	ASN
1	A	294	ASN
1	A	312	GLN
1	A	315	GLN
1	A	375	GLN
1	A	521	GLN
1	A	522	GLN

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Mol	Chain	Res	Type
1	A	547	GLN
2	B	62	GLN
2	B	91	HIS
2	B	94	HIS
2	B	193	GLN
2	B	209	GLN
2	B	326	GLN
3	R	63	GLN
3	R	72	ASN
3	R	76	GLN
3	R	78	GLN
3	R	96	GLN
3	R	97	HIS
3	R	210	ASN
3	R	225	ASN
3	R	247	ASN
3	R	256	ASN
3	R	280	ASN
3	R	305	HIS
3	R	324	GLN
3	R	336	HIS
3	R	439	ASN
3	R	448	GLN
3	R	468	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
7	FAR	P	1428	-	14,14,14	1.15	2 (14%)	16,16,16	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FAR	P	1428	-	-	6/14/14/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1428	FAR	C9-C8	2.46	1.56	1.51
7	P	1428	FAR	C7-C8	2.00	1.37	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	1428	FAR	C3-C5-C6-C7
7	P	1428	FAR	C11-C12-C13-C14
7	P	1428	FAR	C11-C12-C13-C15
7	P	1428	FAR	C10-C8-C9-C11
7	P	1428	FAR	C7-C8-C9-C11
7	P	1428	FAR	C12-C11-C9-C8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	1428	FAR	3	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	536/567 (94%)	0.16	33 (6%) 20 19	27, 54, 74, 81	0
2	B	318/331 (96%)	0.10	9 (2%) 53 54	26, 55, 68, 79	0
3	R	494/650 (76%)	0.12	28 (5%) 23 22	22, 48, 72, 79	0
4	P	4/4 (100%)	2.36	3 (75%) 0 0	67, 70, 71, 72	0
All	All	1352/1552 (87%)	0.14	73 (5%) 25 24	22, 52, 73, 81	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PHE	6.3
3	R	531	ILE	5.7
1	A	78	THR	5.2
1	A	123	PRO	4.8
3	R	210	ASN	4.7
1	A	44	LEU	4.4
2	B	32	SER	4.3
3	R	72	ASN	4.1
3	R	532	GLU	4.1
2	B	331	SER	4.0
1	A	121	PRO	3.9
3	R	304	GLU	3.7
3	R	70	THR	3.7
1	A	83	GLU	3.6
2	B	31	GLY	3.6
2	B	29	SER	3.5
1	A	241	PRO	3.5
3	R	479	PRO	3.4
3	R	409	GLU	3.3
3	R	107	ASP	3.3
1	A	41	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	R	71	GLU	3.2
1	A	84	GLU	3.2
1	A	24	LYS	3.1
1	A	200	GLN	3.1
3	R	480	GLY	3.0
3	R	209	LYS	3.0
4	P	11[A]	ALA	3.0
2	B	11	LYS	3.0
4	P	10[A]	ALA	2.9
1	A	358	VAL	2.9
1	A	45	ASP	2.9
3	R	609	GLU	2.9
1	A	102	VAL	2.9
3	R	600	ASP	2.9
3	R	608	PRO	2.8
1	A	157	ALA	2.8
1	A	77	GLU	2.7
1	A	29	GLN	2.7
1	A	79	GLU	2.7
3	R	411	ARG	2.6
3	R	539	GLU	2.6
3	R	464	ASP	2.6
1	A	42	GLY	2.6
3	R	307	ASP	2.6
1	A	239	ALA	2.6
1	A	30	SER	2.5
1	A	240	GLU	2.5
3	R	598	ASN	2.5
1	A	43	GLU	2.5
3	R	530	GLU	2.5
3	R	64	GLU	2.5
3	R	65	ASN	2.5
1	A	101	ARG	2.5
1	A	440	TYR	2.4
2	B	81	GLU	2.4
1	A	59	ASN	2.4
1	A	176	SER	2.4
1	A	122	GLU	2.3
2	B	278	PHE	2.3
3	R	614	ASP	2.2
4	P	12[A]	ALA	2.2
2	B	304	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	R	310	ARG	2.2
1	A	40	GLN	2.2
1	A	85	SER	2.1
3	R	81	GLU	2.1
3	R	211	ARG	2.1
1	A	68	CYS	2.1
2	B	285	MET	2.1
1	A	38	LYS	2.0
3	R	306	PRO	2.0
1	A	50	GLU	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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
7	FAR	P	1428	15/15	0.68	0.40	63,65,67,67	1
6	CL	R	901	1/1	0.97	0.13	45,45,45,45	0
5	ZN	B	900	1/1	0.98	0.04	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.