



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 8HR0 / pdb_00008hr0
Title : The complex structure of COPII coat with HCoV-OC43 DD sorting motif
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Deposited on : 2022-12-14
Resolution : 3.34 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

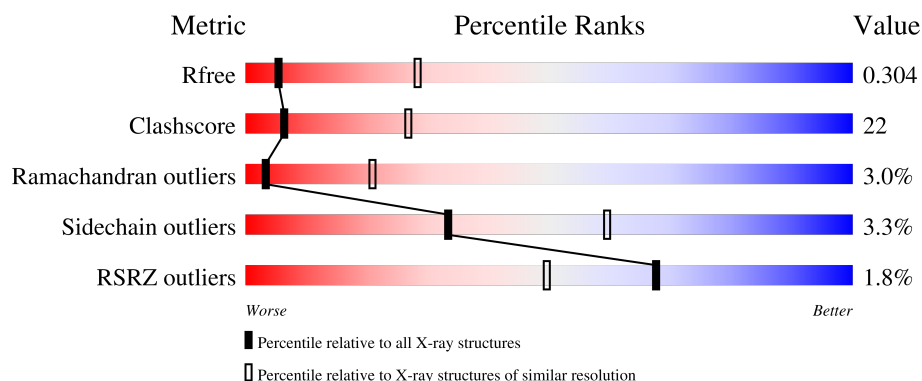
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	765	0% 55% 35% 7%
2	B	751	2% 55% 39% 2%
3	C	199	3% 36% 29% 32%
4	D	10	10% 10% 10% 70%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12401 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 transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5594	3569	964	1023	38			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5717	3651	971	1062	33			

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	135	Total	C	N	O	S	0	0	0
			1066	685	172	201	8			

- Molecule 4 is a protein called HCoV-OC43.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			22	11	3	8			

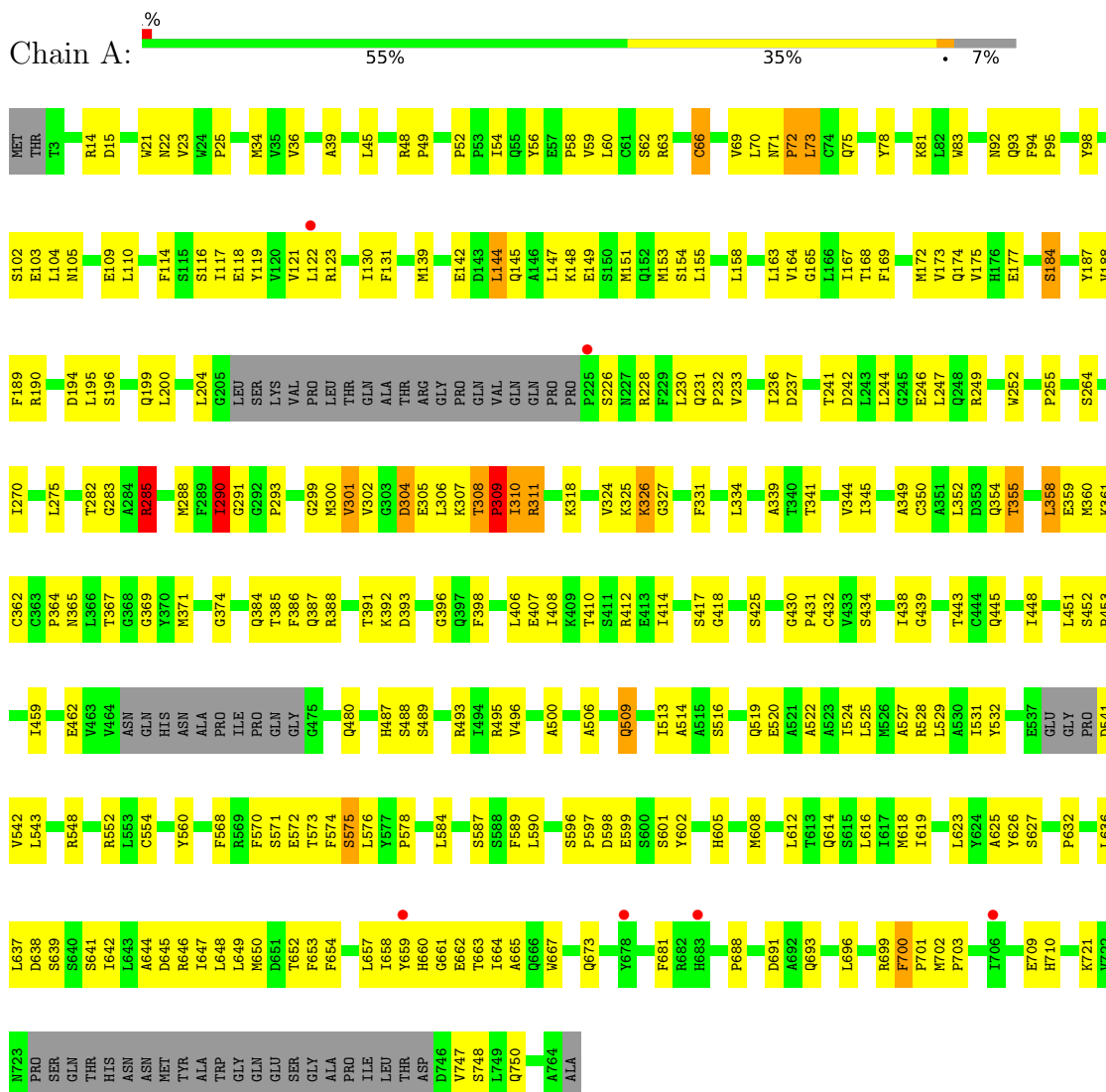
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)

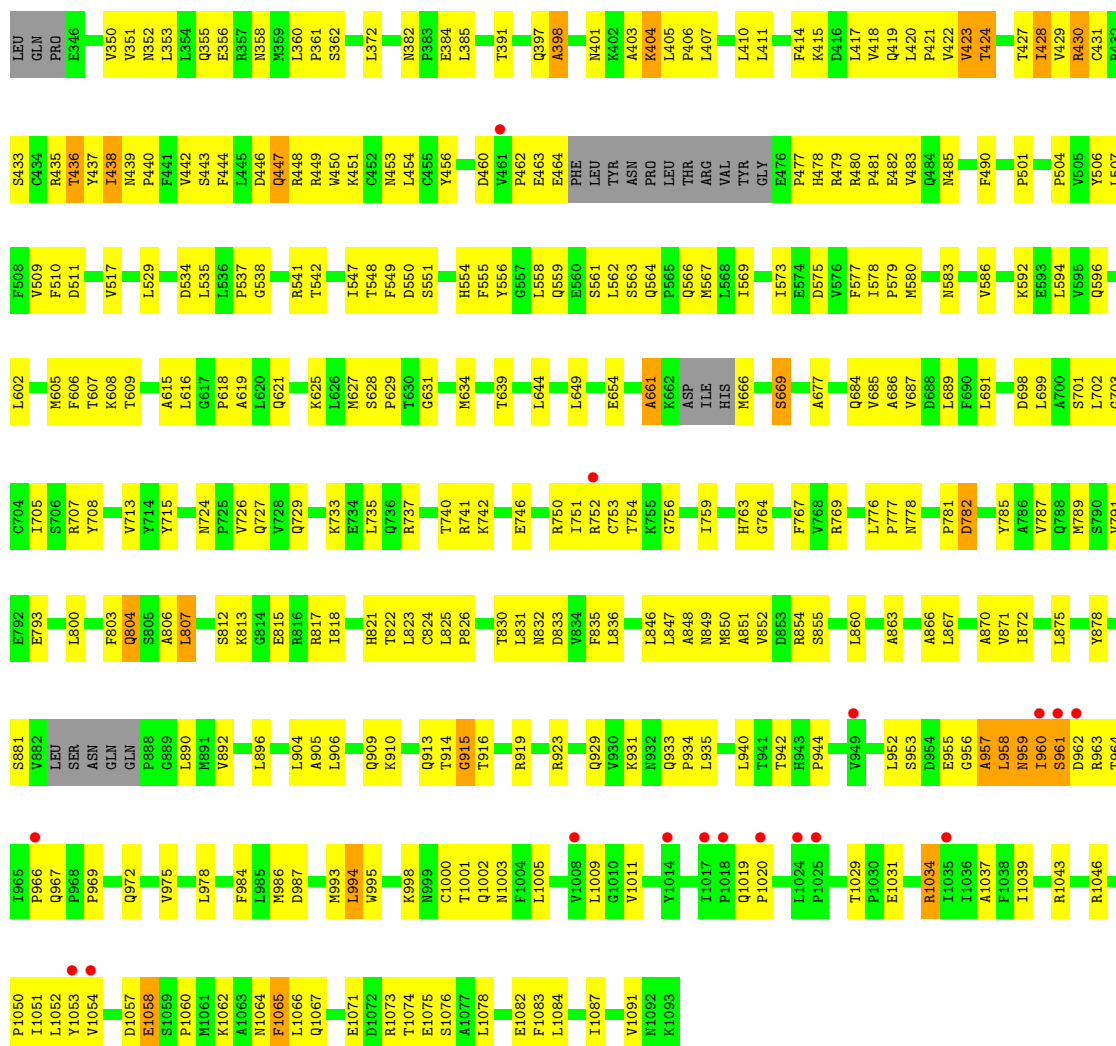
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein Sec23A

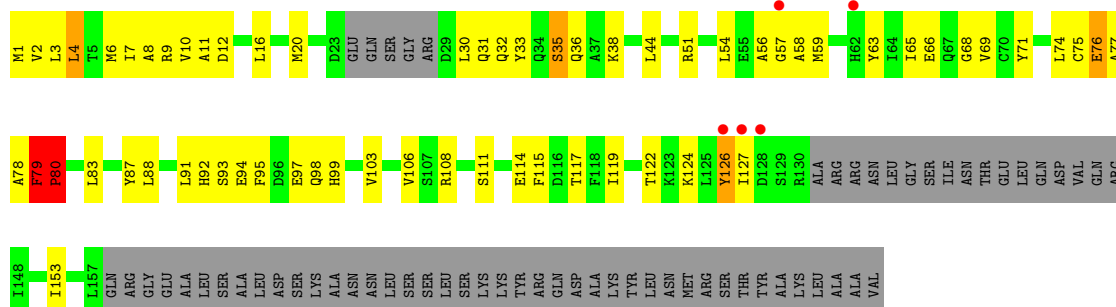


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: HCoV-OC43



GLU	LEU	VAL	ILE	LYS	THR	SER	H527	D528	D529
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.58Å 96.20Å 130.47Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	49.02 – 3.34 49.02 – 3.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.02-3.34) 98.3 (49.02-3.34)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.16.3549	Depositor
R, R_{free}	0.223 , 0.299 0.230 , 0.304	Depositor DCC
R_{free} test set	1994 reflections (7.41%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12401	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.74	3/5725 (0.1%)	0.92	10/7753 (0.1%)
2	B	0.61	0/5839	0.86	2/7940 (0.0%)
3	C	0.45	0/1085	0.77	4/1465 (0.3%)
4	D	0.97	0/21	3.12	4/26 (15.4%)
All	All	0.66	3/12670 (0.0%)	0.89	20/17184 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	C-O	-5.87	1.16	1.23
1	A	290	ILE	C-O	-5.47	1.18	1.24
1	A	364	PRO	C-O	-5.32	1.17	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	528	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	285	ARG	CB-CA-C	-6.97	98.59	110.16
2	B	433	SER	CA-C-N	6.44	131.48	120.72
2	B	433	SER	C-N-CA	6.44	131.48	120.72
4	D	527	HIS	CA-C-N	6.39	134.05	121.58
4	D	527	HIS	C-N-CA	6.39	134.05	121.58
1	A	341	THR	CB-CA-C	5.88	120.11	110.88
1	A	305	GLU	CB-CA-C	-5.81	100.17	109.75
3	C	3	LEU	CA-C-N	5.81	132.63	121.54
3	C	3	LEU	C-N-CA	5.81	132.63	121.54
4	D	529	ASP	CB-CA-C	-5.48	99.69	110.10
1	A	308	THR	CA-C-O	-5.34	115.01	119.76
1	A	334	LEU	N-CA-C	-5.30	105.58	111.36
1	A	572	GLU	CA-C-N	5.30	127.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	GLU	C-N-CA	5.30	127.39	120.28
1	A	309	PRO	N-CA-CB	-5.30	97.68	103.25
3	C	79	PHE	CA-C-N	5.15	126.28	119.84
3	C	79	PHE	C-N-CA	5.15	126.28	119.84
1	A	293	PRO	N-CA-C	5.13	118.41	111.22
1	A	285	ARG	CG-CD-NE	-5.12	100.74	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5594	0	5528	232	0
2	B	5717	0	5737	260	0
3	C	1066	0	1045	63	0
4	D	22	0	9	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12401	0	12319	547	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 22.

All (547) 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:B:454:LEU:HD23	2:B:752:ARG:HG2	1.25	1.17
1:A:644:ALA:O	1:A:664:ILE:HD13	1.45	1.16
2:B:454:LEU:CD2	2:B:752:ARG:HG2	1.76	1.15
2:B:1002:GLN:HA	2:B:1005:LEU:HD12	1.46	0.98
3:C:59:MET:SD	3:C:76:GLU:HA	2.04	0.97
1:A:506:ALA:HA	1:A:509:GLN:HG3	1.50	0.92
1:A:310:ILE:HD12	1:A:310:ILE:H	1.36	0.89
1:A:200:LEU:HD21	1:A:270:ILE:HG23	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:741:ARG:HD2	2:B:781:PRO:HG2	1.56	0.88
1:A:412:ARG:H	1:A:412:ARG:HD3	1.38	0.87
1:A:304:ASP:OD1	1:A:304:ASP:N	2.08	0.87
1:A:487:HIS:HD1	1:A:489:SER:HG	1.19	0.87
2:B:1039:ILE:HD13	2:B:1052:LEU:HD22	1.55	0.86
2:B:726:VAL:HG23	2:B:1053:TYR:OH	1.75	0.86
3:C:59:MET:SD	3:C:76:GLU:CA	2.64	0.85
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.58	0.84
2:B:846:LEU:HG	2:B:850:MET:HE2	1.62	0.82
1:A:168:THR:HG21	1:A:247:LEU:HD11	1.62	0.81
2:B:372:LEU:HD21	2:B:800:LEU:HD21	1.62	0.81
1:A:354:GLN:OE1	1:A:597:PRO:HD2	1.82	0.80
2:B:615:ALA:HB1	2:B:618:PRO:HG2	1.63	0.79
1:A:300:MET:N	1:A:326:LYS:HZ3	1.79	0.79
2:B:956:GLY:HA3	2:B:966:PRO:HA	1.65	0.79
2:B:436:THR:CG2	2:B:454:LEU:HD22	2.14	0.78
3:C:59:MET:HA	3:C:77:ALA:H	1.47	0.78
3:C:2:VAL:O	3:C:79:PHE:HE2	1.66	0.78
2:B:847:LEU:HA	2:B:850:MET:HE3	1.67	0.77
2:B:372:LEU:HG	2:B:826:PRO:HG3	1.68	0.76
3:C:59:MET:SD	3:C:76:GLU:N	2.59	0.76
1:A:139:MET:HG3	1:A:144:LEU:HB2	1.66	0.76
2:B:436:THR:HG23	2:B:752:ARG:HD2	1.67	0.76
1:A:354:GLN:HG2	1:A:598:ASP:OD2	1.85	0.76
2:B:958:LEU:O	2:B:960:ILE:N	2.20	0.75
2:B:1043:ARG:HG2	2:B:1050:PRO:HD2	1.68	0.75
3:C:79:PHE:HD1	3:C:79:PHE:H	1.31	0.75
2:B:1009:LEU:HD21	2:B:1054:VAL:HG11	1.67	0.75
3:C:9:ARG:NH2	3:C:106:VAL:O	2.20	0.74
1:A:103:GLU:OE2	1:A:104:LEU:N	2.20	0.74
2:B:436:THR:HG21	2:B:454:LEU:HD22	1.70	0.74
1:A:300:MET:N	1:A:326:LYS:NZ	2.36	0.74
1:A:290:ILE:HD11	1:A:349:ALA:HB2	1.69	0.74
2:B:806:ALA:HB3	4:D:529:ASP:OD2	1.88	0.73
1:A:300:MET:O	1:A:326:LYS:NZ	2.21	0.73
1:A:310:ILE:HD12	1:A:310:ILE:N	2.03	0.73
3:C:35:SER:OG	3:C:36:GLN:N	2.18	0.73
2:B:446:ASP:C	2:B:448:ARG:H	1.97	0.73
2:B:592:LYS:O	2:B:596:GLN:HG3	1.90	0.71
1:A:647:ILE:HD13	1:A:659:TYR:O	1.90	0.71
2:B:830:THR:HG23	2:B:833:ASP:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ILE:HG13	1:A:667:TRP:CZ2	2.26	0.71
2:B:430:ARG:NH1	2:B:435:ARG:O	2.23	0.71
2:B:958:LEU:CD1	2:B:964:THR:HA	2.21	0.71
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.43	0.71
2:B:602:LEU:HA	2:B:605:MET:HG3	1.72	0.71
2:B:959:ASN:O	2:B:961:SER:N	2.24	0.71
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.26	0.70
1:A:300:MET:H	1:A:326:LYS:NZ	1.89	0.70
1:A:662:GLU:OE1	1:A:710:HIS:ND1	2.24	0.69
2:B:440:PRO:HB3	2:B:483:VAL:O	1.92	0.69
1:A:301:VAL:HG22	1:A:359:GLU:OE1	1.92	0.69
2:B:353:LEU:HD12	2:B:890:LEU:HD23	1.74	0.69
2:B:480:ARG:NH1	2:B:482:GLU:OE1	2.26	0.69
3:C:4:LEU:HD23	3:C:74:LEU:HD23	1.74	0.69
2:B:978:LEU:HA	2:B:984:PHE:HE2	1.57	0.69
1:A:56:TYR:HE1	1:A:98:TYR:OH	1.76	0.68
2:B:750:ARG:CB	4:D:529:ASP:OXT	2.42	0.68
2:B:806:ALA:CB	4:D:529:ASP:OD2	2.42	0.68
1:A:285:ARG:HA	1:A:344:VAL:HG12	1.76	0.68
2:B:984:PHE:O	2:B:995:TRP:N	2.23	0.68
2:B:987:ASP:OD2	2:B:1046:ARG:NH2	2.27	0.68
2:B:1078:LEU:HD22	2:B:1082:GLU:HB3	1.75	0.68
1:A:190:ARG:HD3	2:B:577:PHE:CD2	2.29	0.68
1:A:196:SER:HB3	1:A:199:GLN:HG3	1.75	0.68
2:B:914:THR:O	2:B:916:THR:N	2.25	0.67
2:B:411:LEU:H	2:B:411:LEU:HD23	1.59	0.67
1:A:204:LEU:O	1:A:228:ARG:NH2	2.27	0.67
2:B:462:PRO:O	2:B:464:GLU:N	2.28	0.67
1:A:665:ALA:HB2	1:A:709:GLU:HB2	1.77	0.66
2:B:501:PRO:O	2:B:541:ARG:NH2	2.24	0.66
2:B:815:GLU:OE1	2:B:817:ARG:NH2	2.29	0.66
2:B:956:GLY:O	2:B:958:LEU:N	2.28	0.66
2:B:442:VAL:HG21	2:B:450:TRP:HB2	1.76	0.66
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.77	0.66
2:B:750:ARG:HB3	4:D:529:ASP:OXT	1.97	0.65
2:B:535:LEU:HB3	2:B:740:THR:HG22	1.78	0.65
3:C:31:GLN:OE1	3:C:31:GLN:N	2.29	0.65
2:B:504:PRO:HG2	2:B:542:THR:HA	1.78	0.65
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.79	0.65
1:A:188:VAL:HG11	2:B:579:PRO:HB3	1.79	0.65
2:B:1064:ASN:O	2:B:1067:GLN:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD12	1:A:358:LEU:O	1.98	0.64
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.79	0.64
2:B:737:ARG:NH2	2:B:782:ASP:OD1	2.29	0.64
2:B:753:CYS:O	2:B:753:CYS:SG	2.54	0.64
1:A:131:PHE:CE1	1:A:285:ARG:HG3	2.34	0.63
2:B:405:LEU:HD11	2:B:896:LEU:HD11	1.81	0.63
1:A:139:MET:CG	1:A:144:LEU:HB2	2.29	0.63
1:A:69:VAL:O	1:A:71:ASN:ND2	2.32	0.63
1:A:584:LEU:HB2	1:A:619:ILE:HD13	1.80	0.63
2:B:686:ALA:HB3	2:B:778:ASN:OD1	1.98	0.63
2:B:978:LEU:HA	2:B:984:PHE:CE2	2.33	0.63
2:B:414:PHE:CD2	2:B:742:LYS:HE2	2.34	0.62
2:B:414:PHE:HB3	2:B:781:PRO:HA	1.81	0.62
3:C:58:ALA:O	3:C:77:ALA:HB2	1.98	0.62
3:C:44:LEU:HD23	3:C:65:ILE:HD11	1.81	0.62
1:A:412:ARG:HD3	1:A:412:ARG:N	2.12	0.62
2:B:752:ARG:HB2	2:B:752:ARG:CZ	2.28	0.62
2:B:451:LYS:HZ1	2:B:456:TYR:HA	1.65	0.61
2:B:972:GLN:NE2	2:B:1071:GLU:OE1	2.33	0.61
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.82	0.61
1:A:548:ARG:HE	1:A:552:ARG:NE	1.99	0.61
2:B:438:ILE:O	2:B:438:ILE:HG23	1.99	0.61
2:B:854:ARG:HG2	2:B:863:ALA:HA	1.83	0.61
1:A:528:ARG:HA	1:A:608:MET:HE1	1.82	0.61
3:C:2:VAL:CG2	3:C:79:PHE:HZ	2.13	0.61
1:A:255:PRO:HB2	3:C:1:MET:SD	2.40	0.61
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.83	0.61
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.83	0.61
2:B:554:HIS:CD2	2:B:569:ILE:HG13	2.36	0.61
1:A:311:ARG:O	1:A:311:ARG:HD3	2.01	0.61
2:B:978:LEU:HD23	2:B:984:PHE:HD2	1.66	0.61
2:B:362:SER:HB2	2:B:969:PRO:HB3	1.82	0.60
2:B:554:HIS:ND1	2:B:567:MET:HE3	2.16	0.60
1:A:121:VAL:HG12	1:A:123:ARG:HG3	1.82	0.60
2:B:807:LEU:O	2:B:818:ILE:HA	2.02	0.60
2:B:913:GLN:OE1	2:B:916:THR:HG21	2.02	0.60
3:C:35:SER:O	3:C:38:LYS:N	2.34	0.60
2:B:914:THR:OG1	2:B:915:GLY:N	2.34	0.60
1:A:189:PHE:HZ	1:A:204:LEU:HD21	1.66	0.60
1:A:627:SER:HB3	1:A:646:ARG:HA	1.83	0.60
2:B:558:LEU:HD12	2:B:594:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG21	1:A:270:ILE:HD12	1.83	0.60
1:A:153:MET:SD	1:A:387:GLN:HB3	2.42	0.59
2:B:449:ARG:NH1	2:B:460:ASP:OD1	2.31	0.59
2:B:510:PHE:HB2	2:B:548:THR:HG22	1.84	0.59
2:B:855:SER:HB3	2:B:863:ALA:HB2	1.84	0.59
1:A:310:ILE:H	1:A:310:ILE:CD1	2.04	0.59
2:B:741:ARG:NH1	2:B:782:ASP:OD2	2.35	0.59
1:A:130:ILE:HG12	1:A:163:LEU:HD12	1.84	0.59
2:B:750:ARG:NE	4:D:529:ASP:OXT	2.32	0.59
1:A:602:TYR:O	1:A:605:HIS:HB3	2.02	0.59
2:B:511:ASP:OD2	2:B:639:THR:OG1	2.21	0.59
3:C:59:MET:HA	3:C:77:ALA:N	2.16	0.59
1:A:200:LEU:HD22	1:A:270:ILE:HG12	1.85	0.59
3:C:2:VAL:HG23	3:C:79:PHE:HZ	1.68	0.59
1:A:165:GLY:HA3	1:A:230:LEU:HD23	1.85	0.58
1:A:645:ASP:O	1:A:664:ILE:HD11	2.02	0.58
2:B:440:PRO:HA	2:B:483:VAL:HG13	1.85	0.58
2:B:958:LEU:HD11	2:B:963:ARG:O	2.03	0.58
3:C:108:ARG:O	3:C:111:SER:OG	2.20	0.58
1:A:673:GLN:HE22	1:A:681:PHE:C	2.11	0.58
1:A:355:THR:O	1:A:355:THR:OG1	2.21	0.58
1:A:541:ASP:OD1	1:A:542:VAL:N	2.27	0.58
2:B:401:ASN:O	2:B:404:LYS:HD2	2.02	0.58
1:A:660:HIS:HB3	1:A:664:ILE:HG22	1.86	0.58
1:A:688:PRO:HA	1:A:691:ASP:HB2	1.85	0.58
2:B:397:GLN:OE1	2:B:791:VAL:N	2.34	0.57
2:B:436:THR:HG23	2:B:454:LEU:HD22	1.85	0.57
2:B:689:LEU:HB3	2:B:713:VAL:HG22	1.85	0.57
2:B:454:LEU:HD23	2:B:752:ARG:CG	2.17	0.57
1:A:650:MET:HE1	1:A:721:LYS:HB2	1.86	0.57
1:A:78:TYR:CD2	1:A:103:GLU:HA	2.40	0.57
1:A:151:MET:O	1:A:154:SER:OG	2.21	0.57
2:B:750:ARG:HE	4:D:529:ASP:C	2.12	0.57
3:C:87:TYR:HE1	3:C:122:THR:HB	1.70	0.57
2:B:634:MET:HE3	2:B:687:VAL:HG22	1.87	0.56
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.87	0.56
2:B:929:GLN:O	2:B:933:GLN:HB2	2.05	0.56
2:B:407:LEU:HG	2:B:789:MET:HG3	1.87	0.56
2:B:559:GLN:HG2	2:B:583:ASN:CG	2.30	0.56
1:A:173:VAL:HG22	1:A:189:PHE:HB2	1.87	0.56
1:A:300:MET:CA	1:A:326:LYS:HZ3	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.40	0.56
2:B:410:LEU:HD12	2:B:935:LEU:HD22	1.87	0.56
3:C:54:LEU:HG	3:C:153:ILE:HA	1.87	0.56
2:B:446:ASP:C	2:B:448:ARG:N	2.64	0.56
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.86	0.56
2:B:1000:CYS:SG	2:B:1001:THR:N	2.79	0.56
1:A:339:ALA:HB2	1:A:367:THR:HG22	1.87	0.56
1:A:514:ALA:O	1:A:573:THR:HG21	2.05	0.56
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.40	0.56
1:A:54:ILE:CG2	1:A:56:TYR:CE2	2.89	0.55
1:A:300:MET:H	1:A:326:LYS:HZ3	1.45	0.55
3:C:51:ARG:NH2	3:C:66:GLU:OE2	2.40	0.55
2:B:986:MET:HE2	2:B:993:MET:HE2	1.88	0.55
3:C:75:CYS:HB2	3:C:79:PHE:CD2	2.40	0.55
2:B:677:ALA:HB2	2:B:705:ILE:HD12	1.89	0.55
3:C:114:GLU:O	3:C:117:THR:HG22	2.07	0.55
2:B:360:LEU:HD12	2:B:361:PRO:HD2	1.89	0.55
2:B:654:GLU:HG3	2:B:919:ARG:HD3	1.89	0.54
1:A:659:TYR:CE2	1:A:661:GLY:HA2	2.42	0.54
2:B:437:TYR:HD1	2:B:804:GLN:OE1	1.90	0.54
2:B:661:ALA:HB1	2:B:860:LEU:HB3	1.89	0.54
2:B:958:LEU:HD11	2:B:964:THR:HA	1.88	0.54
1:A:103:GLU:CD	1:A:104:LEU:H	2.15	0.54
2:B:952:LEU:HB3	2:B:966:PRO:HG3	1.89	0.54
3:C:33:TYR:HD2	3:C:74:LEU:HD21	1.73	0.54
1:A:644:ALA:HB2	1:A:662:GLU:HG2	1.90	0.54
3:C:58:ALA:O	3:C:77:ALA:CB	2.56	0.54
1:A:93:GLN:HG2	1:A:94:PHE:N	2.22	0.54
2:B:962:ASP:OD1	2:B:962:ASP:N	2.35	0.54
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.90	0.54
3:C:8:ALA:HA	3:C:16:LEU:HG	1.90	0.54
2:B:986:MET:HE1	2:B:1065:PHE:HA	1.90	0.54
2:B:430:ARG:HB3	2:B:436:THR:O	2.09	0.53
2:B:987:ASP:CG	2:B:1046:ARG:NH2	2.65	0.53
3:C:9:ARG:NH1	3:C:12:ASP:OD2	2.40	0.53
2:B:414:PHE:CE2	2:B:742:LYS:HE2	2.43	0.53
2:B:606:PHE:O	2:B:608:LYS:N	2.42	0.53
2:B:411:LEU:HD23	2:B:411:LEU:N	2.23	0.53
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.91	0.53
1:A:527:ALA:O	1:A:531:ILE:HG12	2.08	0.53
1:A:641:SER:O	1:A:646:ARG:NH2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HG12	1:A:175:VAL:HA	1.89	0.53
2:B:352:ASN:OD1	2:B:355:GLN:HG2	2.08	0.53
2:B:506:TYR:OH	2:B:537:PRO:O	2.23	0.53
2:B:986:MET:HE2	2:B:993:MET:CE	2.39	0.53
1:A:438:ILE:HD13	1:A:529:LEU:HD21	1.90	0.53
2:B:1074:THR:HG22	2:B:1075:GLU:H	1.74	0.53
2:B:550:ASP:OD1	2:B:551:SER:N	2.42	0.52
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	1.90	0.52
2:B:848:ALA:O	2:B:852:VAL:HG23	2.10	0.52
3:C:115:PHE:O	3:C:119:ILE:HG13	2.09	0.52
1:A:231:GLN:HB2	1:A:236:ILE:HD13	1.91	0.52
2:B:454:LEU:HA	2:B:754:THR:HG23	1.90	0.52
2:B:403:ALA:C	2:B:405:LEU:H	2.17	0.52
1:A:173:VAL:CG2	1:A:189:PHE:HB2	2.40	0.52
2:B:942:THR:O	2:B:944:PRO:HD3	2.10	0.52
1:A:264:SER:HB3	1:A:288:MET:HE1	1.92	0.52
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.09	0.52
1:A:190:ARG:HH11	2:B:577:PHE:HB3	1.75	0.52
2:B:556:TYR:HA	2:B:566:GLN:O	2.10	0.52
2:B:846:LEU:HG	2:B:850:MET:CE	2.39	0.52
3:C:59:MET:CG	3:C:76:GLU:HA	2.40	0.51
2:B:446:ASP:OD2	2:B:449:ARG:HG3	2.10	0.51
3:C:71:TYR:HE1	3:C:95:PHE:HD2	1.58	0.51
1:A:452:SER:HB2	1:A:453:PRO:HD2	1.91	0.51
1:A:653:PHE:CE2	1:A:699:ARG:HD3	2.46	0.51
2:B:952:LEU:HD23	2:B:966:PRO:HG2	1.91	0.51
2:B:957:ALA:HB2	2:B:967:GLN:HE22	1.74	0.51
2:B:1064:ASN:C	2:B:1066:LEU:N	2.68	0.51
3:C:93:SER:O	3:C:97:GLU:HB2	2.10	0.51
2:B:430:ARG:CZ	2:B:435:ARG:O	2.57	0.51
1:A:21:TRP:CE3	1:A:513:ILE:HG22	2.46	0.51
1:A:644:ALA:HA	1:A:661:GLY:HA3	1.91	0.51
1:A:246:GLU:CB	2:B:562:LEU:HD13	2.41	0.51
3:C:95:PHE:CD1	3:C:99:HIS:HB2	2.46	0.51
2:B:867:LEU:HD22	2:B:906:LEU:HD23	1.92	0.51
1:A:174:GLN:HA	1:A:187:TYR:O	2.10	0.51
1:A:308:THR:HG23	1:A:308:THR:O	2.10	0.51
3:C:1:MET:HA	3:C:127:ILE:HG23	1.93	0.51
1:A:626:TYR:N	1:A:647:ILE:O	2.43	0.51
2:B:998:LYS:HD2	2:B:1058:GLU:HG2	1.92	0.51
1:A:554:CYS:HA	1:A:570:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ILE:HG23	2:B:618:PRO:CG	2.42	0.50
1:A:406:LEU:O	1:A:445:GLN:HA	2.11	0.50
1:A:417:SER:HA	1:A:434:SER:HB3	1.91	0.50
1:A:575:SER:O	1:A:578:PRO:HD2	2.10	0.50
1:A:639:SER:HA	1:A:642:ILE:HG12	1.92	0.50
2:B:580:MET:HE3	2:B:583:ASN:HB2	1.93	0.50
2:B:759:ILE:HG23	2:B:787:VAL:CG1	2.41	0.50
3:C:7:ILE:HG21	3:C:95:PHE:CE2	2.46	0.50
1:A:548:ARG:HE	1:A:552:ARG:HE	1.58	0.50
2:B:835:PHE:CZ	2:B:878:TYR:HB2	2.46	0.50
3:C:4:LEU:HD11	3:C:20:MET:HE2	1.93	0.50
3:C:2:VAL:HG23	3:C:79:PHE:CZ	2.47	0.50
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.27	0.50
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.92	0.50
1:A:194:ASP:OD1	1:A:195:LEU:N	2.44	0.50
1:A:184:SER:HB3	2:B:564:GLN:OE1	2.12	0.50
2:B:411:LEU:HD23	2:B:785:TYR:O	2.11	0.50
1:A:519:GLN:OE1	1:A:576:LEU:HB2	2.11	0.50
2:B:422:VAL:HG11	2:B:817:ARG:HH11	1.77	0.50
2:B:987:ASP:OD1	2:B:1046:ARG:NH2	2.45	0.50
1:A:434:SER:OG	1:A:462:GLU:OE1	2.30	0.50
2:B:385:LEU:HD21	2:B:415:LYS:HB3	1.93	0.50
2:B:955:GLU:OE1	2:B:955:GLU:N	2.45	0.50
2:B:509:VAL:HG13	2:B:547:ILE:HG22	1.94	0.49
2:B:1073:ARG:HH21	2:B:1082:GLU:CD	2.19	0.49
1:A:102:SER:HB3	1:A:105:ASN:H	1.76	0.49
2:B:958:LEU:HD12	2:B:964:THR:HA	1.95	0.49
1:A:62:SER:OG	1:A:92:ASN:OD1	2.25	0.49
2:B:767:PHE:CE2	2:B:769:ARG:HG2	2.46	0.49
1:A:354:GLN:CG	1:A:598:ASP:OD2	2.60	0.49
2:B:994:LEU:HD12	2:B:1052:LEU:HD11	1.93	0.49
1:A:233:VAL:CG2	1:A:237:ASP:HB3	2.42	0.49
2:B:482:GLU:N	2:B:482:GLU:OE2	2.45	0.49
1:A:131:PHE:CD1	1:A:285:ARG:HG3	2.48	0.49
2:B:707:ARG:HD2	2:B:708:TYR:CE2	2.47	0.49
1:A:14:ARG:HG3	1:A:48:ARG:NH2	2.27	0.49
2:B:684:GLN:OE1	2:B:746:GLU:HA	2.13	0.49
2:B:431:CYS:HB3	2:B:435:ARG:N	2.28	0.49
2:B:1058:GLU:H	2:B:1060:PRO:HD3	1.77	0.48
3:C:66:GLU:OE1	3:C:92:HIS:NE2	2.46	0.48
1:A:288:MET:HE2	1:A:290:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:PHE:CD1	2:B:823:LEU:HD23	2.48	0.48
1:A:384:GLN:C	1:A:386:PHE:H	2.22	0.48
1:A:625:ALA:HB1	1:A:646:ARG:HD2	1.95	0.48
1:A:233:VAL:HG23	1:A:237:ASP:HB3	1.93	0.48
2:B:418:VAL:HG12	2:B:419:GLN:HG2	1.94	0.48
1:A:60:LEU:HD21	1:A:69:VAL:HG22	1.96	0.48
1:A:98:TYR:OH	1:A:109:GLU:OE2	2.30	0.48
1:A:164:VAL:O	1:A:230:LEU:HA	2.13	0.48
2:B:904:LEU:HD13	2:B:1083:PHE:CG	2.49	0.48
3:C:44:LEU:HD21	3:C:63:TYR:CE2	2.49	0.48
3:C:59:MET:SD	3:C:75:CYS:C	2.97	0.48
1:A:410:THR:HB	1:A:414:ILE:HB	1.96	0.48
1:A:69:VAL:H	1:A:480:GLN:HE22	1.62	0.48
1:A:190:ARG:NH1	2:B:577:PHE:HB3	2.29	0.48
2:B:538:GLY:HA2	2:B:812:SER:HB2	1.96	0.48
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.79	0.48
1:A:388:ARG:HA	1:A:391:THR:HG23	1.95	0.47
1:A:58:PRO:HB3	1:A:119:TYR:CD2	2.48	0.47
1:A:300:MET:C	1:A:326:LYS:HZ3	2.22	0.47
2:B:913:GLN:CD	2:B:916:THR:HG21	2.39	0.47
2:B:958:LEU:HD12	2:B:958:LEU:HA	1.75	0.47
2:B:1034:ARG:O	2:B:1037:ALA:N	2.47	0.47
1:A:614:GLN:HB3	1:A:653:PHE:CE2	2.50	0.47
2:B:831:LEU:HD22	2:B:835:PHE:HE2	1.78	0.47
1:A:139:MET:HE2	1:A:291:GLY:HA3	1.95	0.47
1:A:177:GLU:CD	1:A:228:ARG:HD2	2.39	0.47
1:A:596:SER:OG	1:A:599:GLU:HG3	2.14	0.47
2:B:507:LEU:HB3	2:B:627:MET:HE3	1.95	0.47
1:A:439:GLY:HA2	1:A:532:TYR:CE1	2.49	0.47
2:B:439:ASN:CB	2:B:822:THR:HG21	2.45	0.47
1:A:443:THR:OG1	1:A:445:GLN:O	2.20	0.47
1:A:664:ILE:HG13	1:A:667:TRP:HZ2	1.77	0.47
2:B:666:MET:HE1	2:B:923:ARG:HD2	1.96	0.47
1:A:194:ASP:O	1:A:195:LEU:HD23	2.15	0.46
1:A:519:GLN:HE22	1:A:576:LEU:HD12	1.79	0.46
2:B:442:VAL:HG21	2:B:450:TRP:HE3	1.79	0.46
2:B:958:LEU:CD1	2:B:963:ARG:O	2.62	0.46
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.96	0.46
2:B:478:HIS:CE1	2:B:479:ARG:HH11	2.32	0.46
3:C:124:LYS:C	3:C:126:TYR:H	2.23	0.46
1:A:641:SER:OG	1:A:646:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:LEU:HD12	2:B:420:LEU:HB2	1.98	0.46
2:B:975:VAL:HG23	2:B:978:LEU:HD12	1.96	0.46
1:A:241:THR:HG23	1:A:242:ASP:N	2.31	0.46
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.97	0.46
2:B:398:ALA:O	2:B:401:ASN:N	2.49	0.46
2:B:554:HIS:ND1	2:B:567:MET:CE	2.79	0.46
2:B:621:GLN:O	2:B:625:LYS:HG3	2.15	0.46
2:B:1005:LEU:HA	2:B:1009:LEU:HB2	1.98	0.46
1:A:145:GLN:O	1:A:149:GLU:HG3	2.15	0.46
1:A:519:GLN:NE2	1:A:576:LEU:HD12	2.31	0.46
1:A:22:ASN:N	1:A:516:SER:OG	2.49	0.46
1:A:172:MET:HE2	1:A:252:TRP:HZ2	1.80	0.46
1:A:365:ASN:OD1	1:A:605:HIS:ND1	2.44	0.46
3:C:69:VAL:HG21	3:C:103:VAL:HG11	1.97	0.46
1:A:139:MET:O	1:A:249:ARG:HD3	2.16	0.46
1:A:626:TYR:O	1:A:647:ILE:N	2.33	0.46
2:B:428:ILE:HD11	2:B:490:PHE:HB3	1.98	0.46
2:B:442:VAL:HG23	2:B:451:LYS:O	2.16	0.46
2:B:705:ILE:HD12	2:B:705:ILE:HA	1.60	0.46
2:B:803:PHE:HD1	2:B:823:LEU:HD23	1.81	0.46
1:A:119:TYR:HE2	1:A:496:VAL:HG21	1.81	0.45
1:A:626:TYR:CE2	1:A:632:PRO:HG3	2.51	0.45
1:A:36:VAL:HG11	1:A:522:ALA:HB1	1.98	0.45
2:B:724:ASN:ND2	2:B:727:GLN:HG2	2.32	0.45
3:C:95:PHE:CE1	3:C:99:HIS:HB2	2.50	0.45
1:A:118:GLU:OE2	1:A:493:ARG:NH1	2.49	0.45
2:B:851:ALA:O	2:B:854:ARG:HB3	2.17	0.45
1:A:177:GLU:OE1	1:A:228:ARG:HD2	2.17	0.45
1:A:520:GLU:HB3	1:A:612:LEU:HD11	1.98	0.45
2:B:958:LEU:HD12	2:B:964:THR:O	2.16	0.45
3:C:32:GLN:HG2	3:C:33:TYR:HD1	1.81	0.45
3:C:80:PRO:HB2	3:C:83:LEU:HB2	1.98	0.45
1:A:354:GLN:HG2	1:A:598:ASP:CG	2.42	0.45
1:A:644:ALA:HB1	1:A:663:THR:HG22	1.99	0.45
3:C:20:MET:SD	3:C:30:LEU:HD11	2.57	0.45
1:A:226:SER:HB2	1:A:232:PRO:HD3	1.98	0.45
1:A:246:GLU:HB2	2:B:562:LEU:HD13	1.98	0.45
2:B:424:THR:O	2:B:424:THR:OG1	2.11	0.45
2:B:447:GLN:HE21	2:B:477:PRO:HD2	1.80	0.45
2:B:618:PRO:O	2:B:619:ALA:C	2.59	0.45
3:C:71:TYR:CE1	3:C:95:PHE:HD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:LEU:O	1:A:638:ASP:N	2.49	0.45
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.97	0.45
3:C:20:MET:SD	3:C:30:LEU:HD21	2.56	0.45
1:A:650:MET:CE	1:A:721:LYS:HB2	2.47	0.45
2:B:703:GLY:O	2:B:705:ILE:N	2.49	0.45
2:B:703:GLY:C	2:B:705:ILE:H	2.25	0.45
2:B:703:GLY:C	2:B:705:ILE:N	2.73	0.45
2:B:832:ASN:O	2:B:836:LEU:HG	2.17	0.45
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.99	0.45
1:A:145:GLN:HA	1:A:148:LYS:HD3	1.99	0.45
1:A:673:GLN:NE2	1:A:681:PHE:HB3	2.32	0.45
2:B:1084:LEU:HD23	2:B:1084:LEU:HA	1.74	0.45
3:C:6:MET:HB3	3:C:6:MET:HE2	1.66	0.45
1:A:58:PRO:O	1:A:58:PRO:HG2	2.17	0.44
1:A:653:PHE:HA	1:A:699:ARG:NH1	2.32	0.44
2:B:687:VAL:HG11	2:B:705:ILE:HG13	1.99	0.44
2:B:1005:LEU:HD23	2:B:1009:LEU:HD12	1.99	0.44
1:A:392:LYS:HD3	1:A:396:GLY:O	2.17	0.44
1:A:290:ILE:H	1:A:290:ILE:HG12	1.68	0.44
2:B:431:CYS:HB3	2:B:436:THR:H	1.82	0.44
3:C:124:LYS:C	3:C:126:TYR:N	2.75	0.44
1:A:172:MET:HE2	1:A:252:TRP:CZ2	2.52	0.44
1:A:589:PHE:HZ	1:A:618:MET:HB3	1.83	0.44
2:B:763:HIS:ND1	2:B:849:ASN:HB3	2.33	0.44
1:A:95:PRO:HD2	1:A:98:TYR:HB2	2.00	0.44
1:A:350:CYS:HA	1:A:374:GLY:O	2.18	0.44
2:B:350:VAL:HG12	2:B:351:VAL:H	1.81	0.44
2:B:559:GLN:C	2:B:561:SER:H	2.26	0.44
3:C:88:LEU:HA	3:C:91:LEU:HB2	1.99	0.44
1:A:299:GLY:HA2	1:A:327:GLY:HA2	2.00	0.44
2:B:421:PRO:HG3	2:B:485:ASN:OD1	2.18	0.44
1:A:103:GLU:CD	1:A:104:LEU:N	2.75	0.44
1:A:354:GLN:HE21	1:A:354:GLN:HB2	1.68	0.44
2:B:733:LYS:HD2	2:B:733:LYS:HA	1.74	0.44
1:A:623:LEU:HD11	1:A:648:LEU:HD22	2.00	0.44
2:B:480:ARG:HG2	2:B:481:PRO:HD2	2.00	0.44
2:B:812:SER:OG	2:B:813:LYS:HE2	2.17	0.44
3:C:93:SER:OG	3:C:94:GLU:N	2.50	0.44
1:A:109:GLU:H	1:A:109:GLU:HG2	1.36	0.44
1:A:418:GLY:HA3	1:A:438:ILE:O	2.18	0.43
2:B:578:ILE:HA	2:B:579:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HD3	1:A:311:ARG:HH11	1.64	0.43
2:B:940:LEU:CD1	2:B:1046:ARG:HH12	2.31	0.43
2:B:995:TRP:HB2	2:B:1065:PHE:CZ	2.53	0.43
2:B:1057:ASP:N	2:B:1060:PRO:HG3	2.32	0.43
2:B:905:ALA:HB1	2:B:942:THR:HG22	1.98	0.43
3:C:79:PHE:HD1	3:C:79:PHE:N	2.07	0.43
1:A:70:LEU:HD11	1:A:110:LEU:HD21	2.00	0.43
1:A:659:TYR:HE2	1:A:661:GLY:HA2	1.83	0.43
2:B:430:ARG:NE	2:B:435:ARG:O	2.51	0.43
2:B:453:ASN:N	2:B:453:ASN:OD1	2.44	0.43
2:B:573:ILE:HD13	2:B:573:ILE:HA	1.80	0.43
2:B:689:LEU:HD21	2:B:702:LEU:HB3	1.99	0.43
2:B:994:LEU:N	2:B:1053:TYR:O	2.51	0.43
3:C:4:LEU:CD2	3:C:74:LEU:HD23	2.45	0.43
1:A:25:PRO:HD3	1:A:34:MET:HE3	2.00	0.43
1:A:116:SER:HA	1:A:496:VAL:O	2.18	0.43
1:A:657:LEU:HD23	1:A:658:ILE:N	2.33	0.43
2:B:431:CYS:O	2:B:435:ARG:HA	2.18	0.43
2:B:764:GLY:HA2	2:B:931:LYS:O	2.17	0.43
1:A:122:LEU:O	1:A:123:ARG:HG2	2.19	0.43
1:A:543:LEU:H	1:A:543:LEU:HD12	1.83	0.43
2:B:691:LEU:HD23	2:B:715:TYR:CE1	2.54	0.43
2:B:1005:LEU:O	2:B:1011:VAL:N	2.48	0.43
1:A:72:PRO:HD3	1:A:109:GLU:O	2.17	0.43
1:A:331:PHE:CE1	1:A:360:MET:HG2	2.54	0.43
1:A:384:GLN:C	1:A:386:PHE:N	2.75	0.43
1:A:398:PHE:HB2	1:A:488:SER:HB2	2.00	0.43
2:B:356:GLU:H	2:B:356:GLU:HG3	1.64	0.43
2:B:1064:ASN:O	2:B:1065:PHE:C	2.61	0.43
1:A:103:GLU:OE2	1:A:104:LEU:HB2	2.19	0.43
1:A:408:ILE:HD11	1:A:459:ILE:HG12	2.01	0.43
2:B:978:LEU:CA	2:B:984:PHE:HE2	2.31	0.43
2:B:358:ASN:HA	2:B:972:GLN:OE1	2.19	0.42
2:B:551:SER:HA	2:B:644:LEU:HD23	2.00	0.42
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.74	0.42
1:A:352:LEU:HD12	1:A:352:LEU:H	1.84	0.42
1:A:541:ASP:CG	1:A:542:VAL:H	2.21	0.42
1:A:584:LEU:HD13	1:A:619:ILE:HD11	2.00	0.42
2:B:975:VAL:O	2:B:978:LEU:N	2.48	0.42
3:C:32:GLN:HG2	3:C:33:TYR:CD1	2.53	0.42
1:A:147:LEU:O	1:A:151:MET:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:CD2	1:A:270:ILE:HG23	2.37	0.42
1:A:311:ARG:H	1:A:311:ARG:HD2	1.84	0.42
1:A:748:SER:OG	1:A:750:GLN:OE1	2.34	0.42
2:B:517:VAL:HG21	2:B:609:THR:HG22	2.02	0.42
2:B:737:ARG:NE	2:B:782:ASP:OD1	2.50	0.42
1:A:425:SER:HA	1:A:443:THR:HG21	2.01	0.42
1:A:448:ILE:HB	1:A:451:LEU:HD23	2.01	0.42
2:B:1064:ASN:O	2:B:1067:GLN:HG2	2.20	0.42
3:C:7:ILE:HG21	3:C:95:PHE:CD2	2.54	0.42
1:A:560:TYR:HB3	1:A:568:PHE:HD1	1.84	0.42
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.37	0.42
1:A:23:VAL:N	1:A:516:SER:OG	2.52	0.42
1:A:344:VAL:HG22	1:A:369:GLY:CA	2.49	0.42
3:C:2:VAL:CG2	3:C:79:PHE:CZ	2.99	0.42
3:C:56:ALA:HB2	3:C:153:ILE:HG21	2.00	0.42
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.54	0.42
1:A:430:GLY:C	1:A:432:CYS:H	2.28	0.42
2:B:756:GLY:HA2	2:B:793:GLU:HB2	2.01	0.42
2:B:866:ALA:O	2:B:870:ALA:N	2.50	0.42
1:A:693:GLN:HA	1:A:696:LEU:HB3	2.01	0.42
2:B:729:GLN:HG3	2:B:1051:ILE:HD12	2.02	0.42
1:A:155:LEU:HD23	1:A:158:LEU:HD12	2.01	0.41
1:A:282:THR:OG1	1:A:283:GLY:N	2.53	0.41
2:B:875:LEU:HD22	2:B:892:VAL:HG12	2.02	0.41
1:A:103:GLU:OE2	1:A:104:LEU:CA	2.68	0.41
1:A:587:SER:HB2	1:A:589:PHE:CD1	2.56	0.41
1:A:590:LEU:HD23	1:A:590:LEU:HA	1.77	0.41
2:B:442:VAL:CG2	2:B:450:TRP:HB2	2.46	0.41
2:B:562:LEU:HD12	2:B:563:SER:H	1.84	0.41
2:B:615:ALA:HA	2:B:644:LEU:O	2.20	0.41
2:B:909:GLN:HG2	2:B:910:LYS:N	2.35	0.41
1:A:54:ILE:HG13	1:A:117:ILE:HD11	2.03	0.41
1:A:290:ILE:HD12	1:A:360:MET:HE1	2.03	0.41
1:A:702:MET:HA	1:A:703:PRO:HD3	1.89	0.41
2:B:958:LEU:HB3	2:B:959:ASN:H	1.68	0.41
1:A:233:VAL:O	1:A:237:ASP:N	2.52	0.41
1:A:244:LEU:H	1:A:244:LEU:HG	1.73	0.41
1:A:361:LYS:HB2	1:A:371:MET:HE1	2.02	0.41
1:A:54:ILE:HG23	1:A:56:TYR:CD2	2.55	0.41
1:A:195:LEU:HD12	1:A:270:ILE:HG12	2.02	0.41
1:A:361:LYS:HD2	1:A:601:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PHE:HB2	1:A:488:SER:CB	2.50	0.41
1:A:700:PHE:O	1:A:702:MET:N	2.53	0.41
1:A:169:PHE:HB2	1:A:173:VAL:HG12	2.03	0.41
2:B:391:THR:O	2:B:826:PRO:HD2	2.20	0.41
2:B:397:GLN:HB2	2:B:791:VAL:O	2.20	0.41
1:A:130:ILE:HG21	1:A:275:LEU:HD21	2.03	0.41
1:A:652:THR:HG22	1:A:654:PHE:H	1.85	0.41
2:B:385:LEU:HD13	2:B:821:HIS:CE1	2.56	0.41
2:B:628:SER:N	2:B:629:PRO:HD2	2.36	0.41
2:B:691:LEU:HD12	2:B:691:LEU:HA	1.86	0.41
2:B:881:SER:O	2:B:881:SER:OG	2.38	0.41
1:A:45:LEU:HB2	1:A:453:PRO:HA	2.03	0.41
2:B:699:LEU:HA	2:B:702:LEU:HB2	2.02	0.41
2:B:707:ARG:HD2	2:B:708:TYR:CZ	2.55	0.41
2:B:759:ILE:HG12	2:B:789:MET:HE2	2.02	0.41
1:A:63:ARG:HG2	1:A:66:CYS:H	1.86	0.41
1:A:71:ASN:OD1	1:A:73:LEU:HB2	2.21	0.41
1:A:164:VAL:HG23	1:A:236:ILE:HD11	2.03	0.41
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.78	0.41
1:A:663:THR:O	1:A:667:TRP:CD1	2.74	0.41
2:B:382:ASN:OD1	2:B:384:GLU:HG2	2.21	0.41
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.55	0.41
2:B:850:MET:HE3	2:B:850:MET:HB2	1.80	0.41
2:B:1002:GLN:O	2:B:1005:LEU:N	2.54	0.41
1:A:78:TYR:CE2	1:A:103:GLU:HA	2.56	0.41
1:A:574:PHE:O	1:A:576:LEU:N	2.53	0.41
2:B:605:MET:HB2	2:B:606:PHE:CE1	2.56	0.41
2:B:669:SER:OG	2:B:701:SER:OG	2.35	0.41
2:B:752:ARG:HB2	2:B:752:ARG:NH1	2.35	0.41
2:B:423:VAL:O	2:B:423:VAL:CG1	2.68	0.40
2:B:529:LEU:HD23	2:B:529:LEU:HA	1.80	0.40
1:A:71:ASN:C	1:A:73:LEU:H	2.29	0.40
1:A:524:ILE:HD11	1:A:616:LEU:HD23	2.02	0.40
2:B:824:CYS:O	2:B:825:LEU:HD23	2.21	0.40
2:B:914:THR:O	2:B:916:THR:HG22	2.21	0.40
2:B:1029:THR:C	2:B:1031:GLU:N	2.79	0.40
2:B:549:PHE:CZ	2:B:616:LEU:HD13	2.57	0.40
1:A:15:ASP:HA	1:A:116:SER:OG	2.21	0.40
2:B:555:PHE:C	2:B:556:TYR:CD1	2.99	0.40
3:C:10:VAL:HG23	3:C:68:GLY:O	2.22	0.40
3:C:94:GLU:OE2	3:C:98:GLN:NE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG21	1:A:270:ILE:CD1	2.49	0.40
2:B:350:VAL:HG12	2:B:351:VAL:N	2.37	0.40
2:B:442:VAL:CG2	2:B:450:TRP:HE3	2.34	0.40
2:B:735:LEU:HD23	2:B:735:LEU:HA	1.60	0.40
3:C:12:ASP:OD1	3:C:12:ASP:N	2.53	0.40
3:C:87:TYR:OH	3:C:119:ILE:O	2.37	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	698/765 (91%)	621 (89%)	61 (9%)	16 (2%)	5	25
2	B	721/751 (96%)	619 (86%)	80 (11%)	22 (3%)	3	20
3	C	129/199 (65%)	100 (78%)	20 (16%)	9 (7%)	1	7
4	D	1/10 (10%)	1 (100%)	0	0	100	100
All	All	1549/1725 (90%)	1341 (87%)	161 (10%)	47 (3%)	3	21

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	SER
1	A	637	LEU
1	A	649	LEU
2	B	404	LYS
2	B	463	GLU
2	B	575	ASP
2	B	957	ALA
2	B	959	ASN
2	B	960	ILE

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Mol	Chain	Res	Type
2	B	1065	PHE
3	C	4	LEU
3	C	11	ALA
3	C	78	ALA
1	A	66	CYS
2	B	661	ALA
2	B	915	GLY
2	B	1034	ARG
2	B	1058	GLU
2	B	1062	LYS
3	C	57	GLY
3	C	76	GLU
3	C	126	TYR
1	A	81	LYS
1	A	385	THR
1	A	393	ASP
2	B	398	ALA
2	B	1076	SER
1	A	49	PRO
1	A	52	PRO
1	A	184	SER
2	B	447	GLN
2	B	607	THR
2	B	958	LEU
2	B	961	SER
3	C	80	PRO
1	A	700	PHE
3	C	35	SER
1	A	309	PRO
1	A	431	PRO
1	A	509	GLN
2	B	934	PRO
2	B	872	ILE
3	C	79	PHE
1	A	747	VAL
2	B	406	PRO
2	B	438	ILE
1	A	72	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	609/666 (91%)	585 (96%)	24 (4%)	28	56
2	B	647/682 (95%)	630 (97%)	17 (3%)	40	63
3	C	114/172 (66%)	112 (98%)	2 (2%)	51	69
4	D	2/10 (20%)	0	2 (100%)	0	0
All	All	1372/1530 (90%)	1327 (97%)	45 (3%)	33	59

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	73	LEU
1	A	75	GLN
1	A	142	GLU
1	A	144	LEU
1	A	285	ARG
1	A	290	ILE
1	A	301	VAL
1	A	302	VAL
1	A	304	ASP
1	A	306	LEU
1	A	307	LYS
1	A	309	PRO
1	A	310	ILE
1	A	311	ARG
1	A	318	LYS
1	A	324	VAL
1	A	325	LYS
1	A	326	LYS
1	A	345	ILE
1	A	355	THR
1	A	358	LEU
1	A	362	CYS
1	A	571	SER

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Mol	Chain	Res	Type
2	B	423	VAL
2	B	424	THR
2	B	427	THR
2	B	428	ILE
2	B	429	VAL
2	B	430	ARG
2	B	436	THR
2	B	669	SER
2	B	751	ILE
2	B	776	LEU
2	B	777	PRO
2	B	782	ASP
2	B	804	GLN
2	B	807	LEU
2	B	953	SER
2	B	994	LEU
2	B	1003	ASN
3	C	79	PHE
3	C	80	PRO
4	D	528	ASP
4	D	529	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	480	GLN
1	A	519	GLN
1	A	594	ASN
1	A	666	GLN
1	A	673	GLN
1	A	697	HIS
1	A	714	GLN
2	B	447	GLN
2	B	596	GLN
2	B	613	GLN
2	B	683	GLN
2	B	778	ASN
2	B	832	ASN
2	B	849	ASN
2	B	929	GLN
2	B	932	ASN

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Mol	Chain	Res	Type
3	C	39	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	708/765 (92%)	-0.04	6 (0%) 82 69	42, 69, 171, 248	0
2	B	729/751 (97%)	-0.04	17 (2%) 61 42	39, 65, 173, 252	0
3	C	135/199 (67%)	0.65	5 (3%) 45 30	69, 131, 198, 243	0
4	D	3/10 (30%)	1.80	1 (33%) 1 1	21, 21, 23, 30	0
All	All	1575/1725 (91%)	0.02	29 (1%) 67 49	21, 69, 177, 252	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1054	VAL	4.6
2	B	1053	TYR	4.3
3	C	126	TYR	3.1
2	B	1035	ILE	3.0
3	C	128	ASP	2.9
1	A	706	ILE	2.9
3	C	62	HIS	2.7
2	B	461	VAL	2.7
4	D	527	HIS	2.6
2	B	1014	TYR	2.6
2	B	962	ASP	2.6
2	B	960	ILE	2.4
2	B	949	VAL	2.4
2	B	1017	ILE	2.4
2	B	1018	PRO	2.4
1	A	659	TYR	2.3
2	B	1008	VAL	2.3
1	A	678	TYR	2.2
2	B	1025	PRO	2.2
2	B	752	ARG	2.2
1	A	122	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	57	GLY	2.2
1	A	683	HIS	2.2
3	C	127	ILE	2.1
1	A	225	PRO	2.1
2	B	1020	PRO	2.1
2	B	1024	LEU	2.1
2	B	961	SER	2.0
2	B	966	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	ZN	B	1101	1/1	0.96	0.08	76,76,76,76	0
5	ZN	A	801	1/1	1.00	0.02	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.