



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:52 PM UTC

PDB ID : 3KXX / pdb_00003kxx
Title : Structure of the mutant Fibroblast Growth Factor receptor 1
Authors : Bae, J.H.; Boggon, T.J.; Tome, F.; Mandiyan, V.; Lax, I.; Schlessinger, J.
Deposited on : 2009-12-04
Resolution : 3.20 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

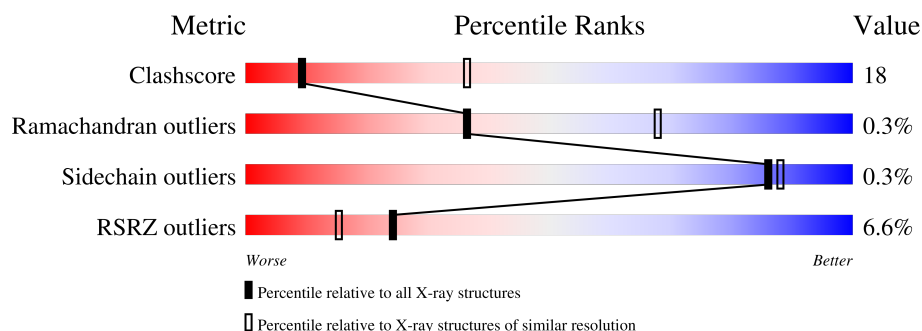
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	317	3% 66% 29% ..
1	B	317	3% 61% 33% ..
1	C	317	11% 54% 36% 10%
1	D	317	8% 52% 39% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9441 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 Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2441	1549	417	458	17			
1	B	305	Total	C	N	O	S	0	0	0
			2438	1549	417	455	17			
1	C	286	Total	C	N	O	S	0	0	0
			2272	1448	388	419	17			
1	D	288	Total	C	N	O	S	0	0	0
			2290	1459	392	421	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	MET	-	expression tag	UNP P11362
A	450	GLY	-	expression tag	UNP P11362
A	451	HIS	-	expression tag	UNP P11362
A	452	HIS	-	expression tag	UNP P11362
A	453	HIS	-	expression tag	UNP P11362
A	454	HIS	-	expression tag	UNP P11362
A	455	HIS	-	expression tag	UNP P11362
A	456	HIS	-	expression tag	UNP P11362
A	457	MET	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	577	GLU	ARG	engineered mutation	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
B	449	MET	-	expression tag	UNP P11362
B	450	GLY	-	expression tag	UNP P11362
B	451	HIS	-	expression tag	UNP P11362
B	452	HIS	-	expression tag	UNP P11362
B	453	HIS	-	expression tag	UNP P11362
B	454	HIS	-	expression tag	UNP P11362
B	455	HIS	-	expression tag	UNP P11362
B	456	HIS	-	expression tag	UNP P11362
B	457	MET	-	expression tag	UNP P11362

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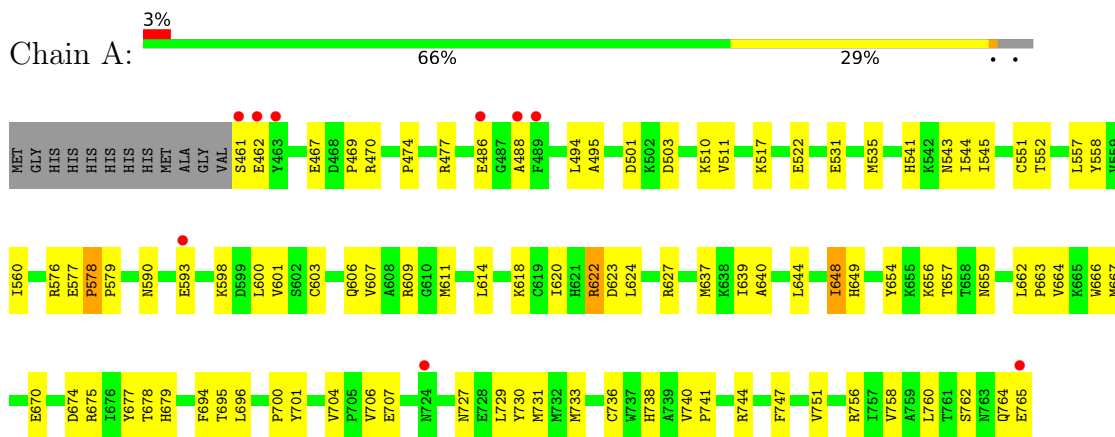
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Chain	Residue	Modelled	Actual	Comment	Reference
B	488	ALA	CYS	engineered mutation	UNP P11362
B	577	GLU	ARG	engineered mutation	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362
C	449	MET	-	expression tag	UNP P11362
C	450	GLY	-	expression tag	UNP P11362
C	451	HIS	-	expression tag	UNP P11362
C	452	HIS	-	expression tag	UNP P11362
C	453	HIS	-	expression tag	UNP P11362
C	454	HIS	-	expression tag	UNP P11362
C	455	HIS	-	expression tag	UNP P11362
C	456	HIS	-	expression tag	UNP P11362
C	457	MET	-	expression tag	UNP P11362
C	488	ALA	CYS	engineered mutation	UNP P11362
C	577	GLU	ARG	engineered mutation	UNP P11362
C	584	SER	CYS	engineered mutation	UNP P11362
D	449	MET	-	expression tag	UNP P11362
D	450	GLY	-	expression tag	UNP P11362
D	451	HIS	-	expression tag	UNP P11362
D	452	HIS	-	expression tag	UNP P11362
D	453	HIS	-	expression tag	UNP P11362
D	454	HIS	-	expression tag	UNP P11362
D	455	HIS	-	expression tag	UNP P11362
D	456	HIS	-	expression tag	UNP P11362
D	457	MET	-	expression tag	UNP P11362
D	488	ALA	CYS	engineered mutation	UNP P11362
D	577	GLU	ARG	engineered mutation	UNP P11362
D	584	SER	CYS	engineered mutation	UNP P11362

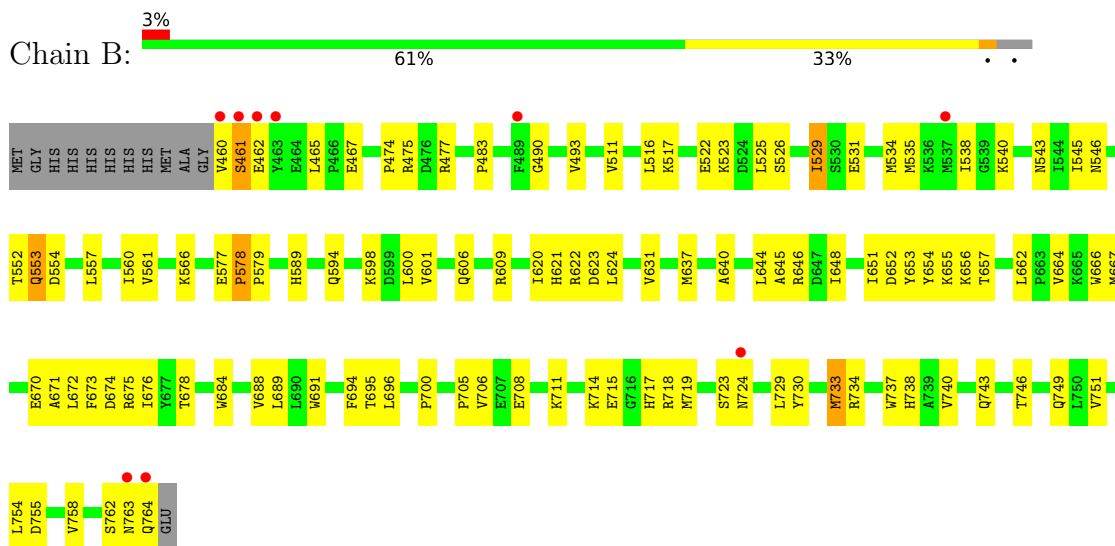
3 Residue-property plots [i](#)

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.

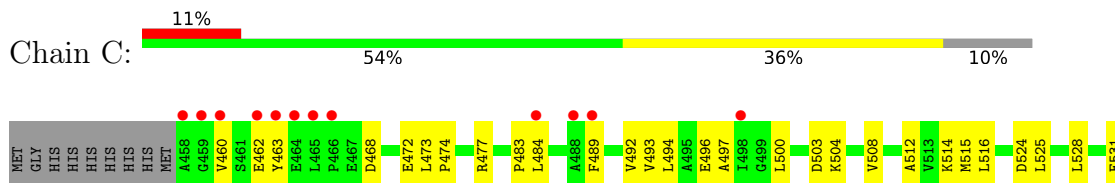
- Molecule 1: Basic fibroblast growth factor receptor 1

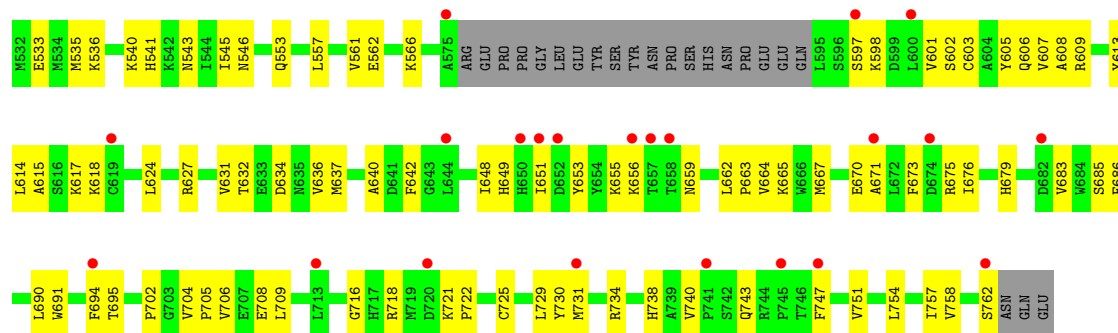


- Molecule 1: Basic fibroblast growth factor receptor 1

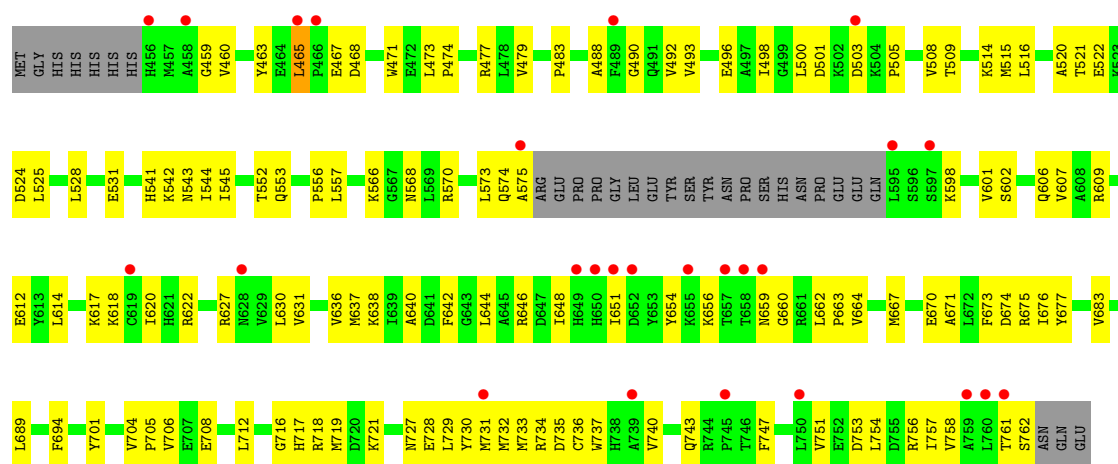


- Molecule 1: Basic fibroblast growth factor receptor 1





● Molecule 1: Basic fibroblast growth factor receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.80Å 74.29Å 135.78Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 96.3 (50.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.263 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9441	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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](#)

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	0.67	0/2496	0.90	4/3376 (0.1%)
1	B	0.67	1/2493 (0.0%)	0.91	5/3374 (0.1%)
1	C	0.48	0/2319	0.80	1/3133 (0.0%)
1	D	0.49	0/2338	0.81	0/3158
All	All	0.59	1/9646 (0.0%)	0.86	10/13041 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	733	MET	SD-CE	-5.92	1.64	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	553	GLN	N-CA-C	7.13	119.72	111.02
1	B	695	THR	N-CA-C	-6.47	104.81	114.64
1	B	553	GLN	N-CA-C	6.30	118.67	111.11
1	A	578	PRO	CA-C-N	6.19	126.09	119.28
1	A	578	PRO	C-N-CA	6.19	126.09	119.28
1	B	578	PRO	CA-C-N	6.01	125.89	119.28
1	B	578	PRO	C-N-CA	6.01	125.89	119.28
1	A	695	THR	N-CA-C	-5.78	104.94	113.61
1	A	644	LEU	N-CA-C	-5.52	106.59	113.38
1	B	673	PHE	N-CA-C	5.12	117.76	111.82

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	2441	0	2429	89	0
1	B	2438	0	2432	82	0
1	C	2272	0	2291	89	0
1	D	2290	0	2307	104	0
All	All	9441	0	9459	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:PRO:HB2	1:D:477:ARG:HG2	1.39	0.99
1:D:664:VAL:HG21	1:D:706:VAL:HG13	1.45	0.98
1:B:664:VAL:HG21	1:B:706:VAL:HG13	1.44	0.98
1:A:664:VAL:HG21	1:A:706:VAL:HG13	1.48	0.95
1:B:531:GLU:HG2	1:B:535:MET:HE2	1.52	0.92
1:C:627:ARG:HH22	1:C:663:PRO:HG3	1.38	0.88
1:D:473:LEU:HD12	1:D:474:PRO:HD2	1.56	0.86
1:D:545:ILE:HD12	1:D:640:ALA:HB2	1.59	0.84
1:A:531:GLU:HG2	1:A:535:MET:HE2	1.58	0.84
1:A:730:TYR:HA	1:A:733:MET:HE3	1.59	0.83
1:C:473:LEU:HD12	1:C:474:PRO:HD2	1.61	0.81
1:C:598:LYS:HB2	1:C:762:SER:HA	1.63	0.79
1:A:664:VAL:HA	1:A:667:MET:HE3	1.64	0.78
1:D:545:ILE:HD11	1:D:630:LEU:HD12	1.65	0.77
1:D:627:ARG:NH2	1:D:663:PRO:HG2	1.99	0.77
1:A:474:PRO:HB2	1:A:477:ARG:HG2	1.66	0.77
1:B:648:ILE:O	1:B:648:ILE:HG22	1.85	0.76
1:C:503:ASP:OD1	1:C:504:LYS:HG2	1.87	0.74
1:A:738:HIS:HD2	1:A:740:VAL:H	1.36	0.73
1:D:521:THR:HG22	1:D:524:ASP:CG	2.13	0.73
1:B:730:TYR:HD1	1:B:733:MET:HE2	1.52	0.73
1:C:627:ARG:NH2	1:C:663:PRO:HG3	2.03	0.73
1:C:655:LYS:HG2	1:C:656:LYS:H	1.54	0.72
1:C:545:ILE:HG13	1:C:640:ALA:HB2	1.71	0.71
1:D:730:TYR:HA	1:D:733:MET:HE3	1.71	0.71
1:A:667:MET:HE1	1:D:522:GLU:HG3	1.74	0.70
1:B:738:HIS:HD2	1:B:740:VAL:H	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:LYS:HE3	1:D:667:MET:HE1	1.72	0.70
1:B:601:VAL:HG12	1:B:758:VAL:HG22	1.73	0.69
1:C:754:LEU:O	1:C:758:VAL:HG23	1.93	0.68
1:C:460:VAL:HG12	1:C:462:GLU:HG3	1.75	0.68
1:B:730:TYR:CD1	1:B:733:MET:HE2	2.29	0.68
1:D:528:LEU:HD23	1:D:557:LEU:HD23	1.76	0.67
1:D:656:LYS:HD2	1:D:677:TYR:HE1	1.58	0.67
1:A:662:LEU:O	1:A:667:MET:HE2	1.97	0.64
1:B:474:PRO:HB2	1:B:477:ARG:HG2	1.78	0.64
1:A:678:THR:HG22	1:A:679:HIS:N	2.13	0.64
1:A:618:LYS:HD2	1:A:649:HIS:ND1	2.14	0.63
1:D:566:LYS:HB2	1:D:631:VAL:HB	1.80	0.63
1:C:664:VAL:HG21	1:C:706:VAL:HG13	1.81	0.62
1:A:486:GLU:HB3	1:A:517:LYS:NZ	2.15	0.62
1:C:516:LEU:HD11	1:C:525:LEU:HD13	1.81	0.62
1:D:754:LEU:O	1:D:758:VAL:HG23	1.99	0.61
1:B:705:PRO:HG2	1:B:708:GLU:HB2	1.81	0.61
1:C:730:TYR:O	1:C:734:ARG:HG2	2.01	0.61
1:A:494:LEU:HD12	1:A:495:ALA:H	1.65	0.59
1:A:579:PRO:HG2	1:A:600:LEU:HD11	1.84	0.59
1:A:627:ARG:NH2	1:A:663:PRO:HG2	2.17	0.59
1:B:598:LYS:HZ1	1:B:762:SER:HB2	1.68	0.59
1:B:578:PRO:HG3	1:B:696:LEU:HD13	1.85	0.59
1:C:492:VAL:HG22	1:C:514:LYS:HG2	1.85	0.59
1:B:516:LEU:HD11	1:B:525:LEU:HD13	1.84	0.59
1:A:664:VAL:HG21	1:A:706:VAL:CG1	2.28	0.58
1:B:694:PHE:CZ	1:B:729:LEU:HD13	2.38	0.58
1:D:492:VAL:HG22	1:D:514:LYS:HG3	1.84	0.58
1:B:579:PRO:HG2	1:B:600:LEU:HD11	1.86	0.58
1:D:753:ASP:HA	1:D:756:ARG:HH22	1.68	0.58
1:A:601:VAL:HG12	1:A:758:VAL:HG22	1.86	0.58
1:B:467:GLU:OE1	1:B:553:GLN:HG3	2.04	0.58
1:D:753:ASP:O	1:D:757:ILE:HG13	2.04	0.58
1:B:738:HIS:HD2	1:B:740:VAL:N	2.02	0.57
1:D:473:LEU:HD12	1:D:474:PRO:CD	2.31	0.57
1:A:701:TYR:HB3	1:A:704:VAL:CG2	2.35	0.57
1:A:477:ARG:HA	1:A:477:ARG:NE	2.19	0.57
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.39	0.57
1:D:730:TYR:O	1:D:734:ARG:HG2	2.04	0.57
1:D:656:LYS:HB3	1:D:675:ARG:HB3	1.85	0.57
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:LEU:O	1:B:758:VAL:HG23	2.04	0.57
1:C:541:HIS:H	1:C:546:ASN:HD21	1.51	0.56
1:D:701:TYR:O	1:D:704:VAL:HG22	2.04	0.56
1:D:543:ASN:ND2	1:D:606:GLN:HB3	2.21	0.56
1:D:503:ASP:O	1:D:505:PRO:HD3	2.06	0.56
1:D:717:HIS:O	1:D:718:ARG:HD2	2.04	0.56
1:A:606:GLN:HB3	1:A:637:MET:HB2	1.88	0.56
1:C:540:LYS:HA	1:C:546:ASN:ND2	2.21	0.56
1:B:462:GLU:HG2	1:C:673:PHE:HD1	1.72	0.55
1:A:477:ARG:HA	1:A:477:ARG:HE	1.69	0.55
1:C:709:LEU:HD23	1:C:709:LEU:O	2.06	0.55
1:A:756:ARG:O	1:A:760:LEU:HG	2.05	0.55
1:A:590:ASN:ND2	1:A:593:GLU:HB3	2.22	0.55
1:C:694:PHE:CZ	1:C:729:LEU:HD13	2.41	0.55
1:D:598:LYS:NZ	1:D:761:THR:HB	2.22	0.55
1:B:526:SER:HB3	1:C:659:ASN:HD22	1.70	0.55
1:D:730:TYR:CZ	1:D:734:ARG:HD3	2.42	0.55
1:A:622:ARG:O	1:A:662:LEU:HD22	2.06	0.55
1:B:545:ILE:HG22	1:B:561:VAL:HB	1.89	0.54
1:A:522:GLU:HB2	1:D:660:GLY:O	2.07	0.54
1:C:533:GLU:OE1	1:C:536:LYS:HE2	2.06	0.54
1:D:474:PRO:HB2	1:D:477:ARG:CG	2.26	0.54
1:A:461:SER:HB3	1:D:659:ASN:HB3	1.88	0.54
1:A:545:ILE:CG1	1:A:640:ALA:HB2	2.38	0.54
1:B:523:LYS:HE3	1:C:659:ASN:O	2.06	0.54
1:C:738:HIS:CD2	1:C:743:GLN:HB2	2.42	0.54
1:B:648:ILE:HG23	1:B:651:ILE:HB	1.89	0.54
1:A:488:ALA:HB2	1:D:488:ALA:HB2	1.90	0.54
1:D:701:TYR:HB3	1:D:704:VAL:HG21	1.90	0.54
1:C:566:LYS:HB2	1:C:631:VAL:O	2.07	0.53
1:C:614:LEU:HD21	1:C:642:PHE:HE1	1.73	0.53
1:C:531:GLU:O	1:C:535:MET:HG2	2.08	0.53
1:D:701:TYR:HB3	1:D:704:VAL:CG2	2.38	0.53
1:C:632:THR:HG22	1:C:636:VAL:H	1.74	0.53
1:A:511:VAL:HG21	1:A:560:ILE:HG23	1.91	0.53
1:B:746:THR:OG1	1:B:749:GLN:HG3	2.09	0.53
1:B:662:LEU:HB2	1:B:667:MET:HE2	1.91	0.53
1:A:470:ARG:HE	1:A:470:ARG:HA	1.75	0.52
1:A:620:ILE:HD11	1:A:648:ILE:HD11	1.90	0.52
1:D:542:LYS:HZ1	1:D:609:ARG:NH1	2.06	0.52
1:C:605:TYR:CZ	1:C:609:ARG:HD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:HIS:HB3	1:A:544:ILE:HG12	1.92	0.52
1:B:738:HIS:CD2	1:B:740:VAL:H	2.24	0.52
1:B:511:VAL:HG21	1:B:560:ILE:HG23	1.91	0.52
1:D:648:ILE:HB	1:D:651:ILE:O	2.10	0.52
1:A:578:PRO:HG3	1:A:696:LEU:HD22	1.92	0.52
1:C:493:VAL:HG22	1:C:515:MET:HE3	1.91	0.52
1:C:601:VAL:HG11	1:C:757:ILE:HG22	1.91	0.52
1:D:566:LYS:HB2	1:D:631:VAL:O	2.09	0.52
1:D:671:ALA:HA	1:D:676:ILE:H	1.74	0.51
1:D:479:VAL:HB	1:D:496:GLU:HB2	1.93	0.51
1:D:500:LEU:HD12	1:D:509:THR:HB	1.92	0.51
1:A:474:PRO:HB2	1:A:477:ARG:CG	2.38	0.51
1:D:598:LYS:HE3	1:D:762:SER:HA	1.92	0.51
1:D:543:ASN:HD22	1:D:606:GLN:HB3	1.76	0.51
1:D:716:GLY:HA2	1:D:718:ARG:NH1	2.26	0.51
1:B:534:MET:HG2	1:B:645:ALA:HB3	1.93	0.51
1:C:738:HIS:CD2	1:C:740:VAL:H	2.27	0.51
1:D:467:GLU:HG2	1:D:553:GLN:NE2	2.26	0.50
1:D:747:PHE:O	1:D:751:VAL:HG23	2.10	0.50
1:A:706:VAL:HG21	1:D:520:ALA:HB3	1.94	0.50
1:B:465:LEU:HD21	1:B:529:ILE:HG12	1.93	0.50
1:B:730:TYR:HA	1:B:733:MET:HG3	1.93	0.50
1:C:503:ASP:O	1:C:504:LYS:HD3	2.11	0.50
1:D:493:VAL:HG22	1:D:515:MET:HE3	1.93	0.50
1:A:738:HIS:CD2	1:A:740:VAL:H	2.25	0.50
1:C:631:VAL:HG22	1:C:637:MET:HE1	1.93	0.50
1:C:603:CYS:O	1:C:607:VAL:HG23	2.12	0.50
1:A:648:ILE:O	1:A:648:ILE:CG2	2.58	0.50
1:A:707:GLU:OE1	1:D:556:PRO:HA	2.11	0.50
1:C:747:PHE:O	1:C:751:VAL:HG23	2.12	0.50
1:A:544:ILE:HG22	1:A:639:ILE:HB	1.94	0.49
1:A:598:LYS:NZ	1:A:762:SER:HB2	2.27	0.49
1:C:662:LEU:HD11	1:C:667:MET:HG2	1.94	0.49
1:D:545:ILE:CD1	1:D:630:LEU:HD12	2.39	0.49
1:D:753:ASP:HA	1:D:756:ARG:NH2	2.27	0.49
1:B:672:LEU:C	1:C:462:GLU:OE2	2.55	0.49
1:C:721:LYS:HZ2	1:C:725:CYS:HB3	1.76	0.49
1:A:494:LEU:HD12	1:A:511:VAL:O	2.12	0.49
1:A:701:TYR:HB3	1:A:704:VAL:HG21	1.95	0.49
1:A:727:ASN:O	1:A:731:MET:HG3	2.13	0.49
1:B:651:ILE:HG22	1:B:652:ASP:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:SER:O	1:D:606:GLN:HG3	2.12	0.49
1:B:545:ILE:HG13	1:B:640:ALA:HB2	1.95	0.49
1:D:717:HIS:C	1:D:718:ARG:HD2	2.38	0.49
1:D:758:VAL:O	1:D:762:SER:HB2	2.12	0.49
1:D:465:LEU:O	1:D:465:LEU:HD12	2.12	0.49
1:A:494:LEU:HD11	1:A:510:LYS:HG3	1.95	0.48
1:B:589:HIS:HE1	1:B:594:GLN:NE2	2.12	0.48
1:B:670:GLU:HG2	1:B:671:ALA:N	2.27	0.48
1:C:632:THR:HG23	1:C:634:ASP:H	1.78	0.48
1:D:490:GLY:HA2	1:D:516:LEU:HA	1.95	0.48
1:A:747:PHE:O	1:A:751:VAL:HG23	2.13	0.48
1:A:678:THR:HG22	1:A:679:HIS:H	1.78	0.48
1:C:540:LYS:HA	1:C:546:ASN:HD22	1.77	0.48
1:B:674:ASP:O	1:B:676:ILE:HG13	2.14	0.48
1:B:461:SER:O	1:B:462:GLU:HB3	2.13	0.48
1:B:684:TRP:CE3	1:B:737:TRP:HA	2.48	0.48
1:B:490:GLY:HA2	1:B:517:LYS:HG3	1.95	0.47
1:D:483:PRO:HA	1:D:493:VAL:HG12	1.96	0.47
1:C:545:ILE:HA	1:C:562:GLU:OE1	2.14	0.47
1:C:602:SER:O	1:C:606:GLN:HG3	2.14	0.47
1:C:632:THR:CG2	1:C:636:VAL:HB	2.44	0.47
1:A:486:GLU:HB3	1:A:517:LYS:HZ3	1.79	0.47
1:A:627:ARG:HH22	1:A:663:PRO:HG2	1.79	0.47
1:B:566:LYS:HB2	1:B:631:VAL:O	2.14	0.47
1:A:461:SER:CB	1:D:659:ASN:HB3	2.45	0.47
1:B:483:PRO:HA	1:B:493:VAL:HA	1.96	0.47
1:C:497:ALA:CB	1:C:500:LEU:HG	2.44	0.47
1:B:656:LYS:HE2	1:B:675:ARG:HA	1.95	0.47
1:B:477:ARG:HA	1:B:477:ARG:NE	2.29	0.47
1:B:631:VAL:HG13	1:B:637:MET:HE1	1.97	0.47
1:B:672:LEU:HG	1:C:462:GLU:OE2	2.15	0.47
1:B:552:THR:HG22	1:B:557:LEU:CD1	2.44	0.47
1:B:714:LYS:HE3	1:C:463:TYR:CE1	2.50	0.46
1:D:541:HIS:HB3	1:D:544:ILE:HD12	1.97	0.46
1:D:570:ARG:O	1:D:574:GLN:HG3	2.15	0.46
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.30	0.46
1:B:460:VAL:HA	1:C:659:ASN:OD1	2.15	0.46
1:C:663:PRO:O	1:C:667:MET:HG3	2.16	0.46
1:A:662:LEU:HD13	1:A:677:TYR:OH	2.16	0.46
1:A:656:LYS:HG3	1:A:657:THR:O	2.16	0.46
1:A:656:LYS:HG2	1:A:675:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:531:GLU:HG3	1:D:642:PHE:HB2	1.98	0.46
1:D:712:LEU:HD13	1:D:717:HIS:ND1	2.30	0.46
1:B:543:ASN:ND2	1:B:606:GLN:HB3	2.31	0.46
1:B:711:LYS:O	1:B:715:GLU:HG2	2.15	0.46
1:C:566:LYS:HB2	1:C:631:VAL:HB	1.98	0.46
1:C:731:MET:HA	1:C:731:MET:HE2	1.97	0.46
1:D:607:VAL:HG11	1:D:689:LEU:HD21	1.97	0.46
1:D:727:ASN:O	1:D:731:MET:HG2	2.15	0.46
1:B:577:GLU:HA	1:B:578:PRO:HD3	1.87	0.46
1:B:671:ALA:HA	1:B:676:ILE:H	1.80	0.46
1:B:475:ARG:NH2	1:B:554:ASP:O	2.49	0.45
1:C:543:ASN:HD22	1:C:606:GLN:HB3	1.81	0.45
1:D:501:ASP:OD1	1:D:503:ASP:HB2	2.15	0.45
1:A:543:ASN:ND2	1:A:606:GLN:HB3	2.32	0.45
1:B:609:ARG:HG2	1:B:609:ARG:HH11	1.81	0.45
1:D:573:LEU:C	1:D:575:ALA:H	2.23	0.45
1:D:636:VAL:C	1:D:637:MET:HE2	2.42	0.45
1:A:741:PRO:HG2	1:B:652:ASP:OD2	2.16	0.45
1:B:651:ILE:HG22	1:B:653:TYR:H	1.81	0.45
1:D:460:VAL:HG11	1:D:525:LEU:HG	1.99	0.45
1:D:721:LYS:HG3	1:D:730:TYR:HB2	1.99	0.45
1:A:701:TYR:O	1:A:704:VAL:HG22	2.16	0.45
1:D:543:ASN:C	1:D:544:ILE:HG13	2.42	0.45
1:D:670:GLU:O	1:D:674:ASP:HB2	2.16	0.45
1:A:531:GLU:CG	1:A:535:MET:HE2	2.39	0.45
1:A:611:MET:SD	1:A:614:LEU:HD12	2.57	0.45
1:D:566:LYS:HG3	1:D:631:VAL:HG12	1.99	0.45
1:D:683:VAL:HG12	1:D:736:CYS:HB3	1.97	0.45
1:A:674:ASP:OD1	1:B:655:LYS:HD2	2.17	0.45
1:B:646:ARG:HG3	1:B:654:TYR:CZ	2.52	0.45
1:D:705:PRO:HB2	1:D:708:GLU:HG3	1.98	0.45
1:B:522:GLU:HB2	1:C:659:ASN:HA	1.98	0.45
1:A:545:ILE:HG12	1:A:640:ALA:HB2	1.98	0.45
1:A:656:LYS:HE2	1:D:522:GLU:OE2	2.16	0.45
1:C:605:TYR:O	1:C:608:ALA:HB3	2.17	0.45
1:A:603:CYS:O	1:A:607:VAL:HG23	2.17	0.45
1:C:512:ALA:HB3	1:C:561:VAL:HG23	1.99	0.45
1:C:648:ILE:HD11	1:C:679:HIS:NE2	2.31	0.45
1:C:705:PRO:HG2	1:C:708:GLU:HB2	1.98	0.45
1:D:516:LEU:HG	1:D:528:LEU:HD22	1.98	0.45
1:D:644:LEU:HD13	1:D:662:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:LYS:HD3	1:D:675:ARG:HA	1.98	0.45
1:A:678:THR:CG2	1:A:679:HIS:N	2.80	0.44
1:B:620:ILE:HD11	1:B:678:THR:HA	1.99	0.44
1:D:704:VAL:O	1:D:704:VAL:HG23	2.17	0.44
1:A:618:LYS:HD2	1:A:649:HIS:CE1	2.52	0.44
1:D:646:ARG:HG3	1:D:654:TYR:CE1	2.52	0.44
1:D:728:GLU:HG3	1:D:729:LEU:N	2.33	0.44
1:A:462:GLU:OE1	1:D:673:PHE:HA	2.17	0.44
1:C:675:ARG:C	1:C:676:ILE:HD12	2.43	0.44
1:D:477:ARG:HB3	1:D:498:ILE:O	2.16	0.44
1:B:738:HIS:CD2	1:B:743:GLN:HB2	2.53	0.44
1:B:763:ASN:O	1:B:764:GLN:HB2	2.17	0.44
1:D:671:ALA:HA	1:D:676:ILE:N	2.33	0.44
1:A:578:PRO:HA	1:A:696:LEU:HD21	2.00	0.44
1:B:730:TYR:CZ	1:B:734:ARG:HD3	2.52	0.44
1:C:496:GLU:HB3	1:C:508:VAL:CG1	2.48	0.44
1:D:732:MET:HA	1:D:735:ASP:OD2	2.18	0.44
1:D:459:GLY:O	1:D:463:TYR:HB2	2.17	0.44
1:C:484:LEU:HD21	1:C:494:LEU:HB2	2.00	0.44
1:A:578:PRO:HA	1:A:579:PRO:HD3	1.83	0.43
1:C:614:LEU:HD21	1:C:642:PHE:CE1	2.52	0.43
1:D:498:ILE:HG13	1:D:508:VAL:HG22	2.00	0.43
1:A:707:GLU:CD	1:A:707:GLU:H	2.26	0.43
1:B:651:ILE:HG22	1:B:652:ASP:H	1.83	0.43
1:C:702:PRO:C	1:C:704:VAL:H	2.26	0.43
1:B:621:HIS:C	1:B:623:ASP:H	2.27	0.43
1:C:656:LYS:HA	1:C:675:ARG:HH21	1.83	0.43
1:C:716:GLY:HA2	1:C:718:ARG:NH1	2.33	0.43
1:D:740:VAL:HB	1:D:743:GLN:HG2	2.00	0.43
1:B:540:LYS:HB2	1:B:546:ASN:ND2	2.32	0.43
1:C:528:LEU:HD23	1:C:557:LEU:HD23	2.00	0.43
1:D:545:ILE:HG13	1:D:638:LYS:HB3	2.00	0.43
1:A:666:TRP:CZ2	1:A:700:PRO:HG2	2.54	0.43
1:C:632:THR:CG2	1:C:636:VAL:H	2.32	0.43
1:A:552:THR:HG22	1:A:557:LEU:CD1	2.49	0.43
1:D:598:LYS:HZ2	1:D:758:VAL:C	2.26	0.43
1:B:688:VAL:HG13	1:B:719:MET:HE1	2.01	0.43
1:B:578:PRO:HG3	1:B:696:LEU:CD1	2.47	0.43
1:C:709:LEU:HD23	1:C:709:LEU:C	2.44	0.43
1:C:721:LYS:HA	1:C:722:PRO:HD3	1.85	0.43
1:D:740:VAL:HB	1:D:743:GLN:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:CYS:HB2	1:A:558:TYR:HB2	2.01	0.43
1:A:611:MET:HE2	1:A:624:LEU:HD22	2.01	0.43
1:B:751:VAL:O	1:B:755:ASP:HB2	2.19	0.42
1:C:721:LYS:NZ	1:C:725:CYS:HB3	2.34	0.42
1:D:694:PHE:CZ	1:D:729:LEU:HD13	2.53	0.42
1:C:683:VAL:O	1:C:686:PHE:HB3	2.19	0.42
1:D:656:LYS:HD2	1:D:677:TYR:CE1	2.46	0.42
1:D:719:MET:HE3	1:D:737:TRP:CH2	2.54	0.42
1:A:467:GLU:O	1:A:469:PRO:HD3	2.18	0.42
1:D:601:VAL:HG12	1:D:758:VAL:HG22	2.02	0.42
1:A:764:GLN:O	1:A:765:GLU:HG2	2.18	0.42
1:C:615:ALA:HA	1:C:679:HIS:CE1	2.55	0.42
1:C:686:PHE:CE2	1:C:690:LEU:HD11	2.55	0.42
1:D:620:ILE:HD11	1:D:648:ILE:HD13	2.01	0.42
1:C:618:LYS:HB2	1:C:649:HIS:CE1	2.55	0.42
1:A:659:ASN:OD1	1:D:460:VAL:HG23	2.20	0.42
1:A:704:VAL:O	1:A:704:VAL:HG23	2.19	0.42
1:B:666:TRP:CZ2	1:B:700:PRO:HG2	2.54	0.42
1:D:468:ASP:OD2	1:D:471:TRP:HD1	2.02	0.42
1:B:644:LEU:N	1:B:644:LEU:HD12	2.35	0.42
1:C:624:LEU:HB3	1:C:685:SER:HB3	2.02	0.42
1:D:568:ASN:HA	1:D:630:LEU:HA	2.02	0.42
1:D:612:GLU:OE1	1:D:751:VAL:HG21	2.20	0.42
1:D:617:LYS:O	1:D:618:LYS:HB2	2.20	0.42
1:A:462:GLU:O	1:A:462:GLU:HG3	2.20	0.41
1:B:624:LEU:HG	1:B:689:LEU:HD12	2.02	0.41
1:C:651:ILE:HG13	1:C:653:TYR:H	1.85	0.41
1:A:477:ARG:HE	1:A:477:ARG:CA	2.33	0.41
1:A:488:ALA:HB2	1:D:488:ALA:CB	2.49	0.41
1:B:664:VAL:HG21	1:B:706:VAL:CG1	2.32	0.41
1:C:671:ALA:HA	1:C:676:ILE:H	1.85	0.41
1:A:622:ARG:NH1	1:A:654:TYR:HE1	2.18	0.41
1:B:631:VAL:HG13	1:B:637:MET:CE	2.51	0.41
1:C:597:SER:O	1:C:601:VAL:HG23	2.21	0.41
1:A:545:ILE:HG13	1:A:640:ALA:HB2	2.01	0.41
1:B:540:LYS:HB2	1:B:546:ASN:HD22	1.86	0.41
1:C:691:TRP:O	1:C:695:THR:HG23	2.20	0.41
1:D:465:LEU:H	1:D:465:LEU:HG	1.70	0.41
1:A:738:HIS:HD2	1:A:740:VAL:N	2.10	0.41
1:B:717:HIS:O	1:B:718:ARG:NH1	2.47	0.41
1:B:723:SER:O	1:B:724:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ALA:HB1	1:C:500:LEU:HG	2.01	0.41
1:C:670:GLU:CD	1:C:670:GLU:H	2.28	0.41
1:A:670:GLU:O	1:A:674:ASP:HB2	2.21	0.41
1:B:691:TRP:HD1	1:B:733:MET:HE1	1.85	0.41
1:C:483:PRO:HA	1:C:493:VAL:HA	2.03	0.41
1:D:465:LEU:HD13	1:D:552:THR:O	2.21	0.41
1:B:672:LEU:O	1:C:462:GLU:OE2	2.39	0.41
1:C:474:PRO:HG2	1:C:477:ARG:HB2	2.03	0.41
1:C:489:PHE:HB3	1:C:524:ASP:CG	2.46	0.41
1:C:609:ARG:HH11	1:C:609:ARG:HG2	1.86	0.41
1:C:705:PRO:HG2	1:C:708:GLU:CB	2.51	0.41
1:D:614:LEU:HD21	1:D:642:PHE:HE1	1.85	0.41
1:D:664:VAL:HG21	1:D:706:VAL:CG1	2.33	0.41
1:B:534:MET:HE2	1:B:538:ILE:HG13	2.02	0.41
1:B:656:LYS:HG2	1:B:657:THR:N	2.35	0.41
1:D:521:THR:HG22	1:D:524:ASP:OD2	2.21	0.41
1:A:623:ASP:HB2	1:A:662:LEU:CD2	2.51	0.40
1:A:501:ASP:OD1	1:A:503:ASP:HB3	2.21	0.40
1:A:576:ARG:HG3	1:A:576:ARG:HH11	1.87	0.40
1:C:632:THR:HG21	1:C:636:VAL:HB	2.03	0.40
1:A:577:GLU:HA	1:A:578:PRO:HD3	1.91	0.40
1:C:468:ASP:O	1:C:472:GLU:HB2	2.20	0.40
1:C:601:VAL:HG12	1:C:758:VAL:HG22	2.02	0.40
1:C:613:TYR:O	1:C:617:LYS:HG2	2.22	0.40
1:A:736:CYS:O	1:A:744:ARG:HD3	2.20	0.40
1:B:467:GLU:HG3	1:B:553:GLN:HG2	2.03	0.40
1:B:621:HIS:O	1:B:623:ASP:N	2.54	0.40
1:C:664:VAL:HG23	1:C:665:LYS:N	2.36	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	303/317 (96%)	288 (95%)	14 (5%)	1 (0%)	36	68
1	B	303/317 (96%)	287 (95%)	14 (5%)	2 (1%)	18	52
1	C	282/317 (89%)	254 (90%)	28 (10%)	0	100	100
1	D	284/317 (90%)	270 (95%)	13 (5%)	1 (0%)	30	62
All	All	1172/1268 (92%)	1099 (94%)	69 (6%)	4 (0%)	36	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	622	ARG
1	A	622	ARG
1	B	461	SER
1	D	622	ARG

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	268/277 (97%)	267 (100%)	1 (0%)	84	86
1	B	268/277 (97%)	267 (100%)	1 (0%)	84	86
1	C	248/277 (90%)	248 (100%)	0	100	100
1	D	250/277 (90%)	249 (100%)	1 (0%)	84	86
All	All	1034/1108 (93%)	1031 (100%)	3 (0%)	86	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	648	ILE
1	B	529	ILE
1	D	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
1	A	589	HIS
1	A	649	HIS
1	A	738	HIS
1	B	589	HIS
1	B	679	HIS
1	B	680	GLN
1	B	724	ASN
1	B	738	HIS
1	C	546	ASN
1	C	574	GLN
1	C	738	HIS
1	D	546	ASN
1	D	574	GLN
1	D	606	GLN
1	D	628	ASN
1	D	659	ASN
1	D	679	HIS
1	D	749	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	305/317 (96%)	0.01	9 (2%)	52 33	12, 39, 83, 97	0
1	B	305/317 (96%)	0.04	9 (2%)	52 33	14, 39, 84, 98	0
1	C	286/317 (90%)	0.87	34 (11%)	9 6	29, 80, 115, 125	0
1	D	288/317 (90%)	0.82	26 (9%)	15 10	28, 74, 111, 122	0
All	All	1184/1268 (93%)	0.42	78 (6%)	24 15	12, 58, 106, 125	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	LEU	5.9
1	D	760	LEU	4.2
1	C	575	ALA	4.1
1	C	458	ALA	4.0
1	D	655	LYS	3.8
1	B	764	GLN	3.8
1	D	489	PHE	3.8
1	D	619	CYS	3.8
1	A	462	GLU	3.7
1	D	575	ALA	3.7
1	C	619	CYS	3.6
1	B	489	PHE	3.5
1	C	762	SER	3.5
1	D	649	HIS	3.5
1	B	460	VAL	3.4
1	A	765	GLU	3.4
1	C	464	GLU	3.2
1	B	462	GLU	3.1
1	A	489	PHE	3.1
1	D	761	THR	3.1
1	D	739	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	460	VAL	3.0
1	C	720	ASP	3.0
1	A	463	TYR	3.0
1	C	463	TYR	3.0
1	C	747	PHE	2.9
1	C	488	ALA	2.9
1	C	459	GLY	2.9
1	D	652	ASP	2.9
1	C	489	PHE	2.9
1	C	656	LYS	2.9
1	B	763	ASN	2.8
1	C	651	ILE	2.8
1	C	745	PRO	2.8
1	D	658	THR	2.8
1	D	650	HIS	2.7
1	C	657	THR	2.7
1	B	724	ASN	2.7
1	D	657	THR	2.6
1	C	650	HIS	2.6
1	C	652	ASP	2.6
1	A	724	ASN	2.6
1	D	465	LEU	2.6
1	B	463	TYR	2.5
1	C	466	PRO	2.5
1	C	644	LEU	2.5
1	C	462	GLU	2.5
1	D	458	ALA	2.5
1	C	674	ASP	2.4
1	A	488	ALA	2.4
1	C	600	LEU	2.4
1	D	750	LEU	2.4
1	D	759	ALA	2.4
1	D	597	SER	2.3
1	D	731	MET	2.3
1	C	597	SER	2.3
1	C	741	PRO	2.2
1	D	745	PRO	2.2
1	B	537	MET	2.2
1	C	713	LEU	2.2
1	A	461	SER	2.2
1	D	503	ASP	2.2
1	C	694	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	671	ALA	2.2
1	C	484	LEU	2.2
1	D	595	LEU	2.2
1	D	456	HIS	2.2
1	A	486	GLU	2.1
1	A	593	GLU	2.1
1	D	628	ASN	2.1
1	D	659	ASN	2.1
1	C	682	ASP	2.1
1	D	651	ILE	2.1
1	C	731	MET	2.1
1	C	498	ILE	2.0
1	D	466	PRO	2.0
1	B	461	SER	2.0
1	C	658	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.