



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:48 PM UTC

PDB ID : 3O4X / pdb_00003o4x
Title : Crystal structure of complex between amino and carboxy terminal fragments of mDia1
Authors : Eck, M.J.; Nezami, A.; Toms, A.V.
Deposited on : 2010-07-27
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:

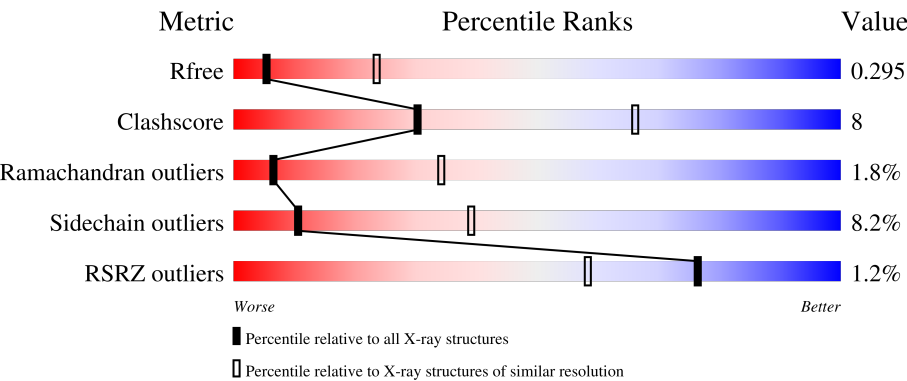
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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))
R _{free}	180053	1466 (3.20-3.20)
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	330	0.2% 69% 25% • •
1	B	330	0.2% 70% 23% • •
1	C	330	0.2% 70% 21% • 6%
1	D	330	2% 75% 19% • •
2	E	467	68% 20% • 7%

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Mol	Chain	Length	Quality of chain
2	F	467	2% 71% 20% • 7%
2	G	467	2% 68% 21% • 7%
2	H	467	% 70% 19% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24335 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 diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2552	1605	440	485	22			
1	B	318	Total	C	N	O	S	0	0	0
			2559	1609	441	487	22			
1	C	311	Total	C	N	O	S	0	0	0
			2508	1579	432	475	22			
1	D	319	Total	C	N	O	S	0	0	0
			2568	1614	442	490	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	expression tag	UNP O08808
A	130	SER	-	expression tag	UNP O08808
B	129	GLY	-	expression tag	UNP O08808
B	130	SER	-	expression tag	UNP O08808
C	129	GLY	-	expression tag	UNP O08808
C	130	SER	-	expression tag	UNP O08808
D	129	GLY	-	expression tag	UNP O08808
D	130	SER	-	expression tag	UNP O08808

- Molecule 2 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	H	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	G	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	F	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	734	GLY	-	expression tag	UNP O08808
E	735	SER	-	expression tag	UNP O08808
H	734	GLY	-	expression tag	UNP O08808
H	735	SER	-	expression tag	UNP O08808
G	734	GLY	-	expression tag	UNP O08808
G	735	SER	-	expression tag	UNP O08808
F	734	GLY	-	expression tag	UNP O08808
F	735	SER	-	expression tag	UNP O08808

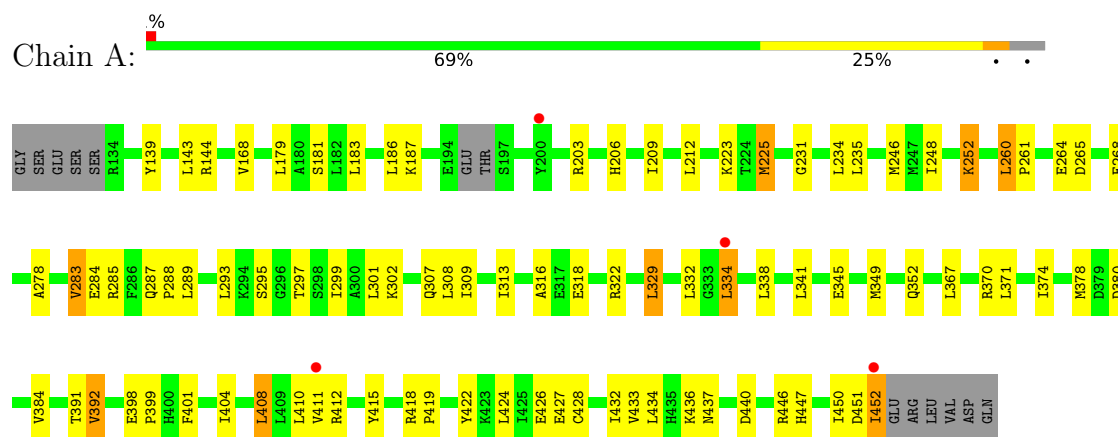
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	6	Total O 6 6	0	0
3	D	8	Total O 8 8	0	0
3	E	5	Total O 5 5	0	0
3	H	4	Total O 4 4	0	0
3	G	6	Total O 6 6	0	0
3	F	2	Total O 2 2	0	0

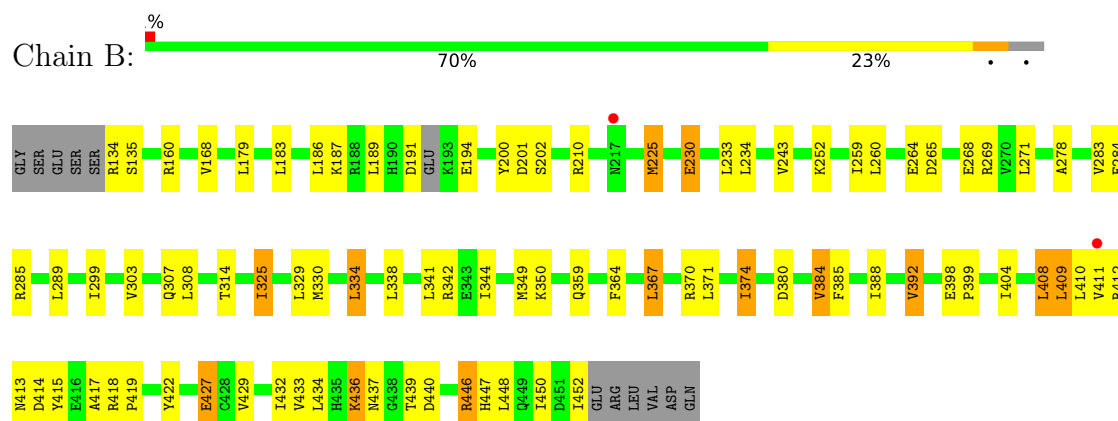
3 Residue-property plots [i](#)

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.

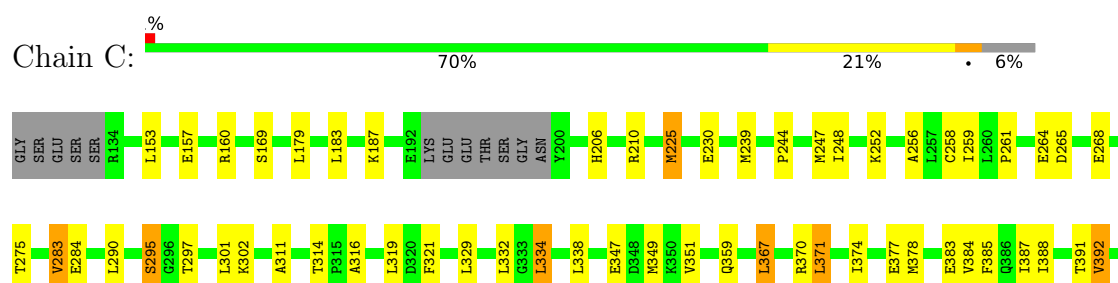
• Molecule 1: Protein diaphanous homolog 1



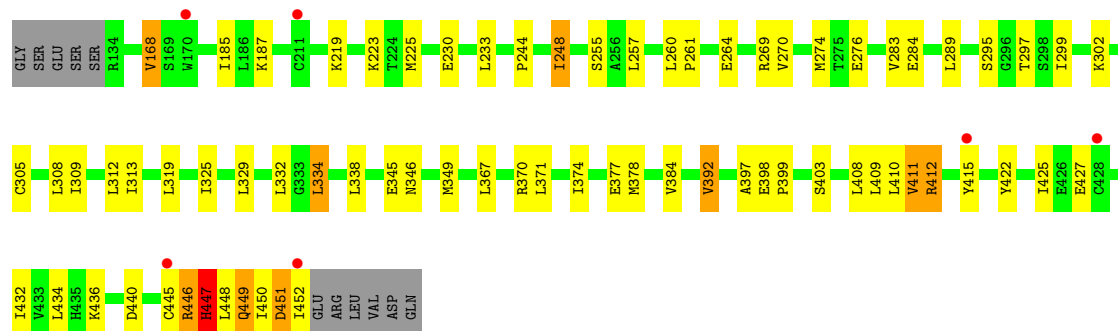
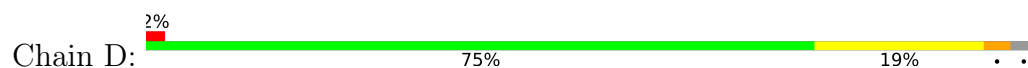
• Molecule 1: Protein diaphanous homolog 1



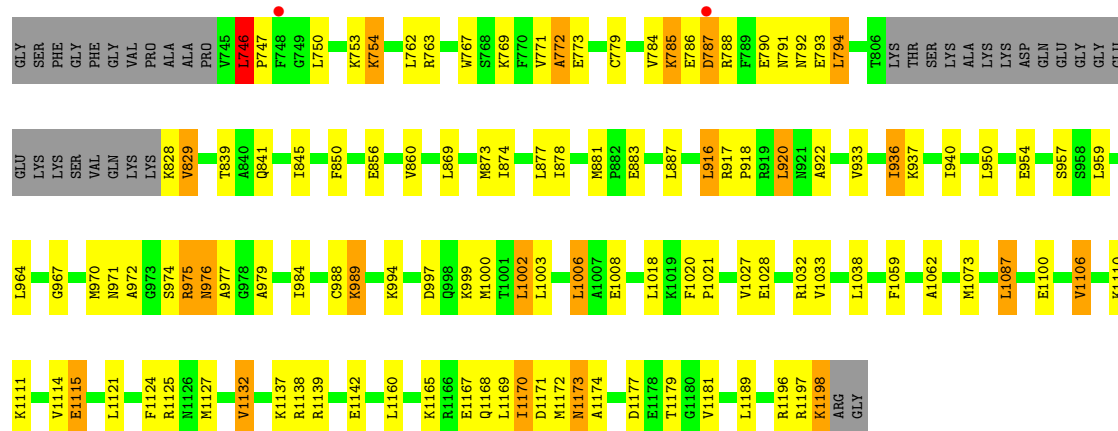
• Molecule 1: Protein diaphanous homolog 1



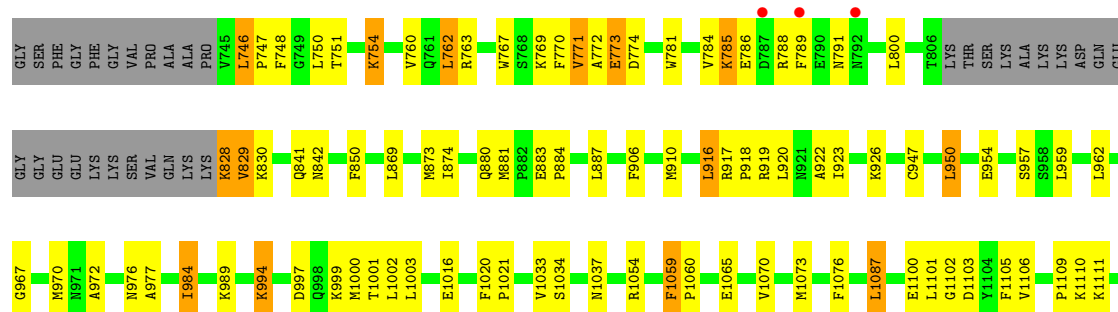
- Molecule 1: Protein diaphanous homolog 1



- Molecule 2: Protein diaphanous homolog 1

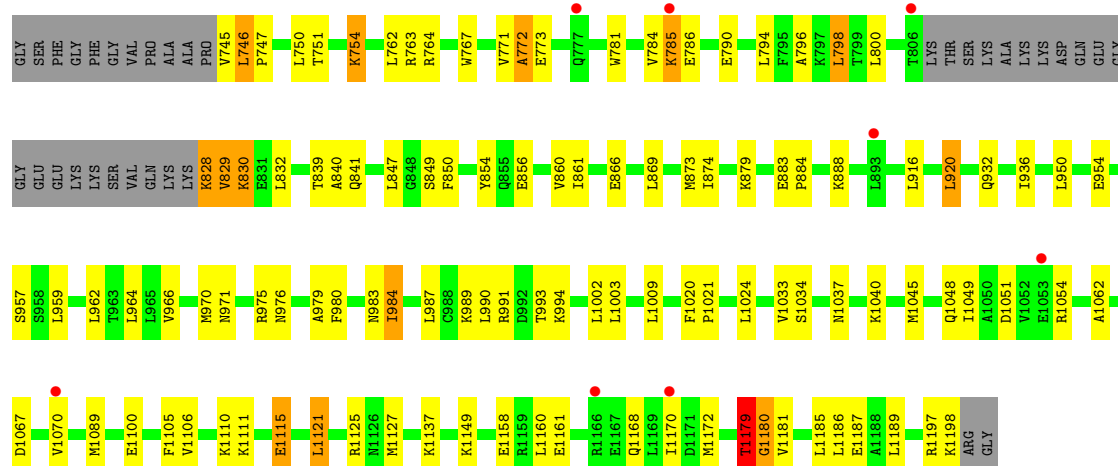


- Molecule 2: Protein diaphanous homolog 1

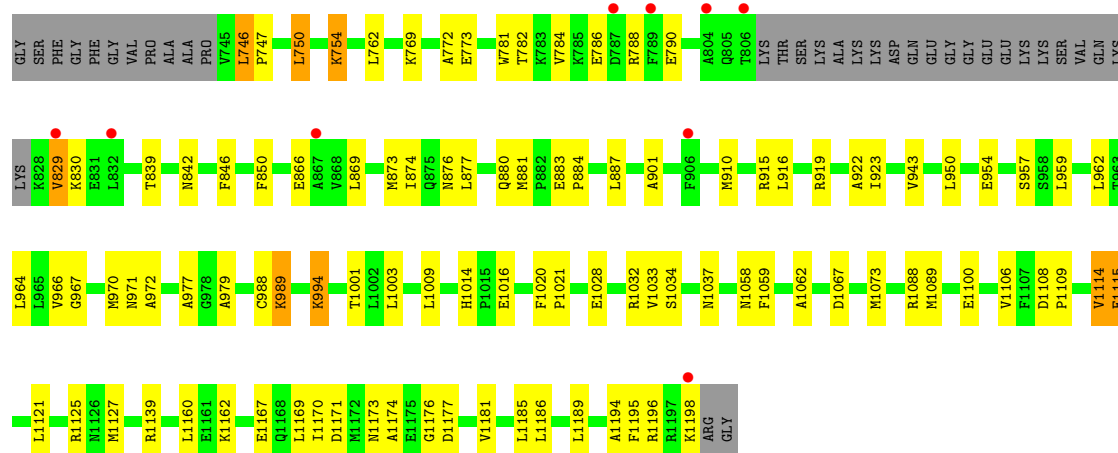




• Molecule 2: Protein diaphanous homolog 1



• Molecule 2: Protein diaphanous homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.76Å 206.83Å 131.06Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	20.12 – 3.20 20.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.12-3.20) 98.6 (20.12-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.233 , 0.298 0.232 , 0.295	Depositor DCC
R_{free} test set	3981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24335	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

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	0.46	0/2588	0.91	2/3483 (0.1%)
1	B	0.45	0/2595	0.88	0/3493
1	C	0.48	0/2544	0.87	0/3425
1	D	0.47	0/2605	0.91	1/3508 (0.0%)
2	E	0.44	0/3580	0.88	1/4799 (0.0%)
2	F	0.44	0/3580	0.87	3/4799 (0.1%)
2	G	0.44	0/3580	0.88	4/4799 (0.1%)
2	H	0.46	0/3580	0.89	5/4799 (0.1%)
All	All	0.45	0/24652	0.89	16/33105 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1174	ALA	N-CA-C	6.73	119.19	111.11
2	H	883	GLU	CA-C-N	6.37	127.80	119.84
2	H	883	GLU	C-N-CA	6.37	127.80	119.84
2	H	785	LYS	N-CA-C	-5.88	106.19	113.19
2	G	883	GLU	CA-C-N	5.88	127.19	119.84
2	G	883	GLU	C-N-CA	5.88	127.19	119.84
1	A	451	ASP	N-CA-C	5.70	119.20	110.20
2	H	751	THR	CA-C-N	5.67	125.68	119.89
2	H	751	THR	C-N-CA	5.67	125.68	119.89
2	G	751	THR	CA-C-N	5.52	126.74	119.84
2	G	751	THR	C-N-CA	5.52	126.74	119.84
1	D	448	LEU	N-CA-C	5.48	117.31	108.32
2	E	1000	MET	N-CA-C	5.34	117.20	108.76
2	F	883	GLU	CA-C-N	5.28	126.44	119.84
2	F	883	GLU	C-N-CA	5.28	126.44	119.84
1	A	295	SER	N-CA-C	5.27	117.77	111.71

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	2552	0	2563	60	0
1	B	2559	0	2570	76	0
1	C	2508	0	2519	58	0
1	D	2568	0	2577	45	0
2	E	3525	0	3552	69	0
2	F	3525	0	3552	60	0
2	G	3525	0	3552	70	0
2	H	3525	0	3552	56	0
3	A	8	0	0	0	0
3	B	9	0	0	1	0
3	C	6	0	0	0	0
3	D	8	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	6	0	0	1	0
3	H	4	0	0	0	0
All	All	24335	0	24437	410	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 8.

All (410) 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:E:988:CYS:HA	2:E:1127:MET:HE1	1.30	1.12
2:F:988:CYS:HA	2:F:1127:MET:HE1	1.48	0.95
1:D:446:ARG:O	1:D:447:HIS:HB2	1.66	0.94
2:G:754:LYS:H	2:G:754:LYS:HE2	1.32	0.94
1:B:410:LEU:HD11	1:C:371:LEU:HB2	1.47	0.94
2:E:828:LYS:N	2:E:829:VAL:HA	1.81	0.92
1:A:248:ILE:HD11	1:A:301:LEU:HA	1.52	0.89
2:E:754:LYS:HE2	2:E:754:LYS:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:CD1	1:A:301:LEU:HA	2.04	0.87
2:H:984:ILE:HD12	2:H:984:ILE:H	1.43	0.83
2:E:1018:LEU:HD21	2:E:1132:VAL:HG21	1.60	0.83
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.42	0.83
2:G:750:LEU:HB2	2:G:785:LYS:HD3	1.59	0.82
2:E:784:VAL:C	2:E:786:GLU:H	1.91	0.78
2:F:754:LYS:HE2	2:F:754:LYS:H	1.49	0.77
2:H:1033:VAL:O	2:H:1115:GLU:HG2	1.84	0.77
2:G:984:ILE:H	2:G:984:ILE:HD12	1.50	0.77
1:D:334:LEU:HD22	1:D:338:LEU:HG	1.66	0.76
2:F:954:GLU:HA	2:F:957:SER:HB3	1.67	0.76
2:E:988:CYS:HA	2:E:1127:MET:CE	2.13	0.75
1:D:451:ASP:HB2	1:D:452:ILE:HG13	1.69	0.75
1:A:265:ASP:HB3	1:A:268:GLU:HG3	1.68	0.75
1:A:378:MET:HB3	1:A:384:VAL:HG22	1.67	0.75
1:A:411:VAL:HG21	1:A:422:TYR:HE1	1.52	0.75
1:C:414:ASP:HB3	1:C:417:ALA:HB3	1.69	0.74
1:B:432:ILE:HD11	1:B:448:LEU:HD21	1.69	0.74
2:G:1033:VAL:O	2:G:1115:GLU:HG2	1.87	0.73
2:E:1002:LEU:HD22	2:E:1006:LEU:HD12	1.71	0.73
1:A:452:ILE:H	1:D:446:ARG:NH1	1.87	0.72
2:F:1088:ARG:HG2	2:F:1088:ARG:HH11	1.54	0.72
1:B:252:LYS:HG2	2:F:1186:LEU:HD22	1.71	0.72
2:G:784:VAL:C	2:G:786:GLU:H	1.94	0.72
1:B:388:ILE:HG12	1:C:409:LEU:HD12	1.70	0.71
1:B:370:ARG:O	1:B:374:ILE:HD13	1.91	0.71
2:E:1033:VAL:O	2:E:1115:GLU:HG2	1.92	0.70
2:H:881:MET:HE1	2:H:887:LEU:HD11	1.73	0.70
2:E:747:PRO:HB3	2:E:772:ALA:HB1	1.73	0.69
1:B:447:HIS:CD2	1:C:449:GLN:HB3	2.27	0.69
1:B:200:TYR:C	1:B:202:SER:H	1.98	0.69
1:D:302:LYS:HB3	1:D:349:MET:HE1	1.75	0.69
2:E:971:ASN:HB3	2:E:976:ASN:O	1.93	0.68
1:A:248:ILE:HD11	1:A:301:LEU:CA	2.23	0.67
2:E:788:ARG:HA	2:E:791:ASN:HD22	1.59	0.67
1:B:283:VAL:HG12	1:B:284:GLU:H	1.59	0.67
2:H:919:ARG:O	2:H:923:ILE:HG12	1.94	0.67
1:B:398:GLU:HB3	1:B:399:PRO:HD3	1.76	0.67
2:H:869:LEU:HD22	2:H:874:ILE:HD11	1.77	0.66
2:E:784:VAL:C	2:E:786:GLU:N	2.54	0.65
2:H:1033:VAL:HG12	2:H:1034:SER:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:CG1	1:C:409:LEU:CD1	2.75	0.65
1:B:427:GLU:HG2	1:B:452:ILE:HG22	1.76	0.65
2:E:763:ARG:O	2:H:970:MET:HE2	1.96	0.65
2:F:994:LYS:HB3	2:F:1001:THR:HG22	1.79	0.65
2:F:869:LEU:HD22	2:F:874:ILE:HD11	1.78	0.64
2:G:794:LEU:HD22	2:F:1009:LEU:HD11	1.78	0.64
2:G:850:PHE:HZ	2:G:873:MET:HG3	1.61	0.64
2:E:922:ALA:HB1	2:E:1073:MET:HE2	1.79	0.64
2:E:1002:LEU:HD22	2:E:1006:LEU:CD1	2.28	0.64
2:F:1033:VAL:O	2:F:1115:GLU:HG2	1.98	0.64
1:B:436:LYS:O	1:B:437:ASN:HB2	1.98	0.63
1:D:168:VAL:HG21	2:H:1177:ASP:HB3	1.79	0.63
2:E:1033:VAL:O	2:E:1115:GLU:CG	2.46	0.63
1:B:200:TYR:C	1:B:202:SER:N	2.56	0.63
1:A:168:VAL:HG11	2:E:1177:ASP:HB3	1.80	0.63
2:G:856:GLU:O	2:G:860:VAL:HG23	1.99	0.63
2:E:786:GLU:C	2:E:788:ARG:H	2.07	0.63
2:G:976:ASN:HA	2:F:769:LYS:HD2	1.82	0.62
1:A:392:VAL:CG1	1:A:398:GLU:HA	2.30	0.62
2:F:1028:GLU:HG2	2:F:1032:ARG:HH21	1.64	0.62
1:B:388:ILE:HG12	1:C:409:LEU:CD1	2.30	0.61
1:C:392:VAL:HG13	1:C:398:GLU:HA	1.83	0.61
1:C:421:TYR:O	1:C:425:ILE:HG12	2.01	0.61
1:B:370:ARG:HG3	1:B:370:ARG:HH11	1.66	0.61
1:B:334:LEU:HD22	1:B:338:LEU:HG	1.82	0.61
2:E:841:GLN:HG3	2:G:1168:GLN:HE22	1.66	0.60
1:A:411:VAL:HG21	1:A:422:TYR:CE1	2.35	0.60
1:C:259:ILE:HD11	2:G:1185:LEU:HD22	1.82	0.60
1:B:283:VAL:HG12	1:B:284:GLU:N	2.16	0.60
1:A:225:MET:HE2	1:A:231:GLY:HA3	1.83	0.59
2:F:1062:ALA:HB1	2:F:1067:ASP:HB3	1.84	0.59
1:C:334:LEU:HD22	1:C:338:LEU:HG	1.83	0.58
2:H:906:PHE:O	2:H:910:MET:HG2	2.03	0.58
1:D:398:GLU:HB3	1:D:399:PRO:HD3	1.85	0.58
1:B:330:MET:HG3	1:B:439:THR:HG21	1.84	0.58
2:G:971:ASN:HB3	2:G:976:ASN:O	2.03	0.58
1:B:299:ILE:HD11	1:B:344:ILE:CG2	2.33	0.58
2:F:994:LYS:HA	2:F:1001:THR:HA	1.86	0.58
2:E:970:MET:HE2	2:H:763:ARG:O	2.04	0.57
2:E:1168:GLN:HE22	2:G:841:GLN:HG3	1.69	0.57
1:A:371:LEU:HB2	1:D:410:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:HG21	1:B:422:TYR:HE1	1.69	0.57
1:B:392:VAL:CG1	1:B:398:GLU:HA	2.33	0.57
1:B:411:VAL:HG21	1:B:422:TYR:CE1	2.40	0.57
2:G:754:LYS:HE2	2:G:754:LYS:N	2.13	0.57
1:C:398:GLU:HB3	1:C:399:PRO:HD3	1.85	0.57
2:H:917:ARG:HB3	2:H:918:PRO:HD3	1.87	0.56
2:G:954:GLU:HA	2:G:957:SER:HB3	1.87	0.56
1:C:383:GLU:O	1:C:387:ILE:HD13	2.05	0.56
2:G:1170:ILE:HG21	2:G:1172:MET:HE2	1.87	0.56
2:E:1198:LYS:HB2	2:E:1198:LYS:NZ	2.20	0.56
2:E:1165:LYS:HG2	2:G:841:GLN:HE21	1.70	0.56
1:B:436:LYS:H	1:B:436:LYS:HD2	1.71	0.56
2:H:828:LYS:O	2:H:829:VAL:HG22	2.06	0.56
1:C:411:VAL:HG21	1:C:422:TYR:HE1	1.71	0.55
1:B:388:ILE:HG13	1:C:409:LEU:CD1	2.36	0.55
1:C:378:MET:HB3	1:C:384:VAL:HG22	1.89	0.55
2:G:1158:GLU:HB3	2:G:1198:LYS:HE2	1.89	0.55
2:F:915:ARG:HH22	2:F:1058:ASN:HB3	1.71	0.55
2:G:829:VAL:O	2:G:830:LYS:HB2	2.07	0.55
1:B:415:TYR:CD2	2:H:989:LYS:HD3	2.41	0.55
1:C:248:ILE:CD1	1:C:301:LEU:HA	2.35	0.55
2:F:784:VAL:C	2:F:786:GLU:H	2.14	0.55
1:A:289:LEU:HD21	1:A:308:LEU:HD23	1.88	0.55
1:A:209:ILE:HA	1:A:212:LEU:HD12	1.88	0.55
1:C:259:ILE:CD1	2:G:1185:LEU:HD22	2.37	0.55
1:C:295:SER:HA	1:C:302:LYS:CE	2.37	0.55
1:A:418:ARG:HB3	1:A:419:PRO:HD3	1.88	0.54
1:A:436:LYS:O	1:A:437:ASN:HB2	2.08	0.54
1:A:380:ASP:O	1:A:384:VAL:HG23	2.07	0.54
1:B:446:ARG:HH11	1:B:446:ARG:CG	2.17	0.54
2:E:954:GLU:HA	2:E:957:SER:HB3	1.88	0.54
2:H:950:LEU:CD1	2:H:1105:PHE:CE1	2.91	0.54
2:F:842:ASN:HB3	2:F:880:GLN:HE22	1.71	0.54
1:A:398:GLU:HB3	1:A:399:PRO:HD3	1.90	0.54
1:B:404:ILE:CD1	1:C:426:GLU:HA	2.38	0.54
1:A:428:CYS:O	1:A:432:ILE:HD13	2.08	0.54
1:B:388:ILE:HG13	1:C:409:LEU:HD11	1.88	0.54
1:C:153:LEU:O	1:C:157:GLU:HB2	2.08	0.54
2:F:919:ARG:O	2:F:923:ILE:HG12	2.07	0.54
2:F:830:LYS:HD3	2:F:901:ALA:HA	1.90	0.54
2:E:1124:PHE:HA	2:E:1127:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:798:LEU:HD11	2:F:966:VAL:HG13	1.89	0.54
2:H:1102:GLY:HA3	2:H:1109:PRO:HG3	1.90	0.53
1:A:401:PHE:HA	1:A:404:ILE:HD12	1.90	0.53
2:H:976:ASN:O	2:H:977:ALA:HB3	2.07	0.53
1:D:370:ARG:O	1:D:374:ILE:HG12	2.07	0.53
2:E:869:LEU:HD22	2:E:874:ILE:HD11	1.90	0.53
2:G:1062:ALA:HB1	2:G:1067:ASP:HB3	1.89	0.53
2:F:922:ALA:HB1	2:F:1073:MET:HE2	1.90	0.53
2:H:788:ARG:HA	2:H:791:ASN:HD22	1.73	0.53
2:E:967:GLY:HA3	2:H:767:TRP:CH2	2.44	0.53
2:E:1171:ASP:C	2:E:1173:ASN:H	2.17	0.53
1:A:179:LEU:HD21	1:A:225:MET:HE3	1.90	0.53
1:A:432:ILE:HG21	1:D:425:ILE:HG13	1.91	0.53
1:B:392:VAL:HG13	1:B:398:GLU:HA	1.90	0.53
2:H:784:VAL:C	2:H:786:GLU:H	2.16	0.53
1:D:450:ILE:O	1:D:451:ASP:O	2.26	0.53
1:A:206:HIS:CD2	1:A:246:MET:HA	2.44	0.52
2:H:1033:VAL:HG12	2:H:1034:SER:N	2.24	0.52
1:C:244:PRO:O	1:C:248:ILE:HG12	2.09	0.52
2:H:784:VAL:C	2:H:786:GLU:N	2.68	0.52
2:E:936:ILE:O	2:E:940:ILE:HG12	2.09	0.52
2:E:1028:GLU:HG2	2:E:1032:ARG:HH21	1.75	0.52
2:H:1034:SER:HB3	2:H:1037:ASN:HB2	1.91	0.52
2:G:832:LEU:HD21	2:G:840:ALA:CB	2.40	0.52
1:B:271:LEU:HD21	1:B:325:ILE:HD11	1.92	0.52
2:H:922:ALA:HB1	2:H:1073:MET:HE2	1.91	0.52
1:A:168:VAL:HG22	2:E:1179:THR:HG23	1.92	0.51
1:A:419:PRO:HA	1:D:397:ALA:HB2	1.91	0.51
1:B:303:VAL:O	1:B:307:GLN:HB2	2.10	0.51
2:G:1024:LEU:HD13	2:G:1121:LEU:HD11	1.92	0.51
1:A:424:LEU:HD23	1:D:432:ILE:HG23	1.92	0.51
1:D:305:CYS:O	1:D:309:ILE:HG12	2.10	0.51
2:H:850:PHE:HZ	2:H:873:MET:HG3	1.74	0.51
1:A:186:LEU:HD23	1:A:234:LEU:HB3	1.92	0.51
1:B:367:LEU:HD12	1:B:434:LEU:HD23	1.92	0.51
1:B:409:LEU:HD13	1:C:388:ILE:HG12	1.93	0.51
1:C:252:LYS:HE3	2:G:1186:LEU:HD13	1.92	0.51
1:A:392:VAL:HG13	1:A:398:GLU:HA	1.92	0.51
1:D:445:CYS:HA	1:D:446:ARG:HH21	1.75	0.51
1:B:371:LEU:HB2	1:C:410:LEU:HD11	1.93	0.51
1:C:347:GLU:O	1:C:351:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ARG:O	1:D:447:HIS:CB	2.46	0.51
2:E:997:ASP:OD1	2:E:999:LYS:HB2	2.11	0.50
2:G:984:ILE:HD12	2:G:984:ILE:N	2.24	0.50
2:H:950:LEU:CD1	2:H:1105:PHE:HE1	2.24	0.50
2:G:763:ARG:O	2:F:970:MET:HE2	2.11	0.50
1:B:440:ASP:CG	1:C:412:ARG:HH21	2.20	0.50
1:C:302:LYS:HB3	1:C:349:MET:HE1	1.92	0.50
2:G:784:VAL:C	2:G:786:GLU:N	2.63	0.50
1:B:168:VAL:HG11	2:F:1177:ASP:HB3	1.93	0.50
1:D:261:PRO:HG3	2:H:1166:ARG:HG2	1.93	0.50
2:F:964:LEU:HD11	2:F:979:ALA:O	2.11	0.50
2:E:940:ILE:HD13	2:E:1038:LEU:HD13	1.94	0.50
2:H:781:TRP:HA	2:H:784:VAL:HG22	1.94	0.50
2:G:964:LEU:HD11	2:G:979:ALA:O	2.12	0.49
1:A:139:TYR:O	1:A:143:LEU:HG	2.12	0.49
1:B:409:LEU:HD11	1:C:387:ILE:HG22	1.94	0.49
2:E:1138:ARG:O	2:E:1142:GLU:HG2	2.11	0.49
2:G:781:TRP:HA	2:G:784:VAL:HG22	1.92	0.49
1:D:168:VAL:HG22	2:H:1179:THR:HG23	1.94	0.49
1:B:450:ILE:O	1:C:446:ARG:HB3	2.13	0.49
2:E:850:PHE:HZ	2:E:873:MET:HG3	1.77	0.49
2:F:988:CYS:HA	2:F:1127:MET:CE	2.30	0.49
1:A:450:ILE:O	1:D:446:ARG:HB2	2.13	0.49
1:B:289:LEU:HD21	1:B:308:LEU:HD23	1.95	0.49
2:G:861:ILE:HD12	2:G:920:LEU:HD11	1.95	0.49
2:H:926:LYS:HA	2:H:1076:PHE:CZ	2.48	0.49
2:G:764:ARG:HD2	2:F:971:ASN:HA	1.95	0.49
1:B:299:ILE:HD11	1:B:344:ILE:HG23	1.95	0.48
2:E:793:GLU:OE1	2:E:793:GLU:HA	2.13	0.48
2:G:790:GLU:HG3	2:F:1014:HIS:CE1	2.48	0.48
1:C:295:SER:HA	1:C:302:LYS:HE3	1.95	0.48
2:G:1020:PHE:CD2	2:G:1021:PRO:HD3	2.49	0.48
1:B:338:LEU:O	1:B:342:ARG:HG3	2.14	0.48
1:B:359:GLN:HE22	2:F:1162:LYS:NZ	2.11	0.48
1:B:429:VAL:HG22	1:C:425:ILE:HG23	1.96	0.48
1:D:255:SER:HB3	2:H:1189:LEU:HD21	1.94	0.48
2:F:754:LYS:HE2	2:F:754:LYS:N	2.23	0.48
2:G:1179:THR:O	2:G:1181:VAL:N	2.46	0.48
2:F:943:VAL:HG11	2:F:1114:VAL:HG11	1.96	0.48
1:A:283:VAL:HG12	1:A:284:GLU:H	1.79	0.48
2:F:1020:PHE:N	2:F:1021:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:LEU:HD21	1:D:308:LEU:HD23	1.95	0.48
1:A:433:VAL:HG11	1:D:410:LEU:HB2	1.94	0.48
1:B:418:ARG:HB3	1:B:419:PRO:HD3	1.96	0.48
2:G:987:LEU:HD23	2:G:990:LEU:HD11	1.96	0.48
1:A:289:LEU:HD13	1:A:309:ILE:HD12	1.96	0.47
2:H:881:MET:CE	2:H:887:LEU:HD11	2.42	0.47
2:F:829:VAL:O	2:F:830:LYS:HB2	2.14	0.47
1:A:334:LEU:HD22	1:A:338:LEU:HG	1.96	0.47
1:D:299:ILE:HD11	1:D:346:ASN:HB2	1.96	0.47
1:A:440:ASP:OD2	1:D:412:ARG:NH2	2.47	0.47
2:E:786:GLU:C	2:E:788:ARG:N	2.72	0.47
2:E:974:SER:O	2:E:975:ARG:C	2.56	0.47
2:H:841:GLN:HE22	2:F:1196:ARG:HG3	1.80	0.47
2:F:754:LYS:H	2:F:754:LYS:CE	2.23	0.47
1:C:265:ASP:HB3	1:C:268:GLU:HG3	1.95	0.47
1:D:270:VAL:O	1:D:274:MET:HG3	2.13	0.47
1:A:144:ARG:HE	1:A:181:SER:HB3	1.78	0.47
1:B:314:THR:HG21	2:F:1195:PHE:HB3	1.96	0.47
1:B:404:ILE:HD11	1:C:426:GLU:N	2.29	0.47
2:G:869:LEU:HD22	2:G:874:ILE:HD11	1.96	0.47
1:B:200:TYR:O	1:B:202:SER:N	2.48	0.47
1:A:302:LYS:HB3	1:A:349:MET:HE1	1.97	0.47
1:B:364:PHE:CD1	1:B:436:LYS:HA	2.50	0.46
1:B:380:ASP:O	1:B:384:VAL:HG23	2.15	0.46
1:B:433:VAL:CG1	1:C:410:LEU:HB3	2.45	0.46
1:D:302:LYS:HB3	1:D:349:MET:CE	2.45	0.46
1:D:378:MET:HB3	1:D:384:VAL:HG22	1.96	0.46
2:E:1106:VAL:HG13	2:H:770:PHE:CE1	2.49	0.46
1:B:413:ASN:OD1	1:B:418:ARG:NH2	2.49	0.46
1:D:230:GLU:HG2	1:D:233:LEU:HD23	1.97	0.46
1:D:319:LEU:HD23	1:D:370:ARG:HH21	1.80	0.46
2:G:1115:GLU:H	2:G:1115:GLU:HG3	1.48	0.46
2:E:786:GLU:O	2:E:788:ARG:N	2.48	0.46
1:C:206:HIS:CE1	1:C:210:ARG:HH21	2.34	0.46
2:G:847:LEU:HD22	2:G:854:TYR:HE1	1.79	0.46
2:G:1048:GLN:HA	2:G:1051:ASP:HB2	1.98	0.46
2:F:846:PHE:CE1	2:F:876:ASN:HB3	2.51	0.46
2:F:874:ILE:HA	2:F:877:LEU:HD12	1.98	0.46
1:B:183:LEU:HD21	1:B:225:MET:HE1	1.98	0.46
2:E:933:VAL:HG13	2:E:1087:LEU:HD21	1.98	0.46
2:E:1008:GLU:HG3	2:E:1139:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:983:ASN:HB3	3:G:44:HOH:O	2.16	0.46
1:A:297:THR:HB	1:A:301:LEU:HD23	1.98	0.46
1:A:313:ILE:O	1:A:322:ARG:HD2	2.15	0.46
1:B:230:GLU:HG3	1:B:233:LEU:HD23	1.96	0.46
1:B:271:LEU:CD2	1:B:325:ILE:HD11	2.45	0.46
2:E:917:ARG:HB3	2:E:918:PRO:HD3	1.98	0.46
2:E:1198:LYS:HE2	2:G:879:LYS:NZ	2.30	0.46
2:G:796:ALA:O	2:G:800:LEU:HG	2.16	0.46
1:D:411:VAL:HG21	1:D:422:TYR:CE1	2.51	0.46
2:E:1170:ILE:HD12	2:E:1172:MET:HG2	1.96	0.46
2:G:767:TRP:CH2	2:F:967:GLY:HA3	2.50	0.46
1:A:452:ILE:H	1:D:446:ARG:HH12	1.60	0.45
1:B:415:TYR:CG	2:H:989:LYS:HD3	2.51	0.45
2:H:754:LYS:HE2	2:H:754:LYS:H	1.81	0.45
2:F:750:LEU:HD22	2:F:782:THR:HG23	1.98	0.45
1:A:293:LEU:HD22	1:A:341:LEU:HD11	1.97	0.45
1:B:186:LEU:HD23	1:B:234:LEU:HB3	1.97	0.45
1:B:412:ARG:NH2	1:C:440:ASP:OD2	2.49	0.45
1:D:392:VAL:HG13	1:D:398:GLU:HA	1.97	0.45
2:E:792:ASN:HB2	2:E:794:LEU:HD23	1.97	0.45
1:C:410:LEU:O	1:C:411:VAL:C	2.59	0.45
1:D:219:LYS:HG3	2:H:1181:VAL:HG21	1.99	0.45
2:E:1018:LEU:CD2	2:E:1132:VAL:HG21	2.40	0.45
2:H:842:ASN:HB3	2:H:880:GLN:HE22	1.81	0.45
2:F:1169:LEU:HD11	2:F:1194:ALA:HA	1.99	0.45
1:B:414:ASP:HB3	1:B:417:ALA:HB3	1.98	0.45
2:E:750:LEU:HB2	2:E:785:LYS:HD3	1.97	0.45
2:E:841:GLN:HG3	2:G:1168:GLN:NE2	2.30	0.45
2:G:1020:PHE:N	2:G:1021:PRO:CD	2.80	0.45
2:F:846:PHE:HE1	2:F:876:ASN:HB3	1.80	0.45
2:E:754:LYS:HD2	2:E:788:ARG:HH21	1.82	0.45
2:E:964:LEU:HD11	2:E:979:ALA:O	2.17	0.45
1:D:244:PRO:O	1:D:248:ILE:HG12	2.17	0.45
2:E:1196:ARG:HG3	2:G:841:GLN:HE22	1.81	0.45
2:H:1197:ARG:O	2:H:1198:LYS:C	2.60	0.45
2:F:1171:ASP:C	2:F:1173:ASN:H	2.25	0.45
2:E:746:LEU:HA	2:E:747:PRO:HD3	1.67	0.45
1:C:239:MET:HB3	1:C:247:MET:HE3	1.99	0.45
1:A:329:LEU:HB3	1:A:334:LEU:HD12	1.99	0.44
2:H:786:GLU:HB3	2:H:789:PHE:HB2	1.99	0.44
2:F:1088:ARG:HG2	2:F:1088:ARG:NH1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:881:MET:HE2	2:E:916:LEU:HD12	1.99	0.44
2:H:910:MET:HE3	2:H:916:LEU:HD11	1.99	0.44
2:F:910:MET:HE3	2:F:916:LEU:HD11	1.99	0.44
1:B:404:ILE:HD11	1:C:426:GLU:HA	1.99	0.44
2:H:747:PRO:HB3	2:H:772:ALA:HB1	2.00	0.44
2:G:767:TRP:HH2	2:F:967:GLY:HA3	1.83	0.44
2:G:771:VAL:O	2:G:772:ALA:C	2.60	0.44
2:G:828:LYS:O	2:G:829:VAL:C	2.59	0.44
2:G:966:VAL:O	2:G:970:MET:HG3	2.18	0.44
2:F:1088:ARG:HH11	2:F:1088:ARG:CG	2.26	0.44
2:H:750:LEU:HB2	2:H:785:LYS:HD3	2.00	0.44
2:H:771:VAL:HG12	2:H:774:ASP:OD2	2.18	0.44
2:G:1034:SER:HB3	2:G:1037:ASN:HB2	2.00	0.44
1:A:248:ILE:O	1:A:252:LYS:HB2	2.17	0.44
1:C:316:ALA:HB1	1:C:321:PHE:HD2	1.83	0.44
1:D:276:GLU:HA	2:G:975:ARG:HD3	2.00	0.44
1:D:295:SER:HA	1:D:302:LYS:CE	2.48	0.44
1:A:261:PRO:HB3	2:E:1167:GLU:HG2	2.00	0.44
1:B:299:ILE:HD11	1:B:344:ILE:HG21	1.99	0.44
2:H:947:CYS:HA	2:H:1101:LEU:HD11	2.00	0.44
1:B:404:ILE:HD13	1:C:426:GLU:HA	2.00	0.44
1:A:183:LEU:HD11	1:A:225:MET:HE1	2.00	0.43
1:C:160:ARG:CD	1:C:210:ARG:HB3	2.48	0.43
2:E:771:VAL:O	2:E:772:ALA:C	2.61	0.43
1:B:134:ARG:HB3	1:B:135:SER:H	1.58	0.43
1:B:189:LEU:C	1:B:191:ASP:H	2.25	0.43
1:B:412:ARG:HH21	1:C:440:ASP:CG	2.26	0.43
2:E:856:GLU:O	2:E:860:VAL:HG23	2.18	0.43
2:E:988:CYS:CA	2:E:1127:MET:HE1	2.22	0.43
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.66	0.43
1:A:410:LEU:O	1:A:411:VAL:C	2.61	0.43
1:B:265:ASP:HB3	1:B:268:GLU:HG3	2.00	0.43
2:F:1020:PHE:CD2	2:F:1021:PRO:HD3	2.54	0.43
1:B:408:LEU:O	1:B:411:VAL:HG22	2.18	0.43
1:C:248:ILE:HD13	1:C:301:LEU:HA	2.00	0.43
1:D:415:TYR:CG	2:F:989:LYS:HD3	2.53	0.43
2:G:991:ARG:HD3	2:G:1127:MET:HG2	1.99	0.43
2:G:993:THR:O	2:G:1002:LEU:HB2	2.19	0.43
1:A:278:ALA:HB2	1:A:285:ARG:HA	2.00	0.43
1:A:412:ARG:NH1	1:D:440:ASP:OD1	2.52	0.43
2:G:1037:ASN:HA	2:G:1040:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1111:LYS:HD3	2:G:1111:LYS:HA	1.82	0.43
1:B:179:LEU:HD21	1:B:225:MET:HE3	2.01	0.43
2:E:767:TRP:CH2	2:H:967:GLY:HA3	2.54	0.43
2:E:976:ASN:HA	2:H:769:LYS:HD2	2.00	0.43
2:F:1185:LEU:O	2:F:1189:LEU:HB2	2.19	0.43
1:B:446:ARG:CG	1:B:446:ARG:NH1	2.80	0.43
1:C:446:ARG:HD2	1:C:446:ARG:N	2.33	0.43
2:E:881:MET:CE	2:E:887:LEU:HD11	2.49	0.43
1:A:415:TYR:HB2	2:G:989:LYS:HD3	2.01	0.42
2:H:1020:PHE:CD2	2:H:1021:PRO:HD3	2.53	0.42
2:F:1167:GLU:C	2:F:1169:LEU:H	2.27	0.42
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.93	0.42
1:A:426:GLU:HG3	1:D:403:SER:HB3	2.00	0.42
1:C:258:CYS:HB3	1:C:311:ALA:O	2.19	0.42
2:F:1108:ASP:HA	2:F:1109:PRO:HD3	1.90	0.42
2:G:980:PHE:O	2:F:781:TRP:HB3	2.19	0.42
2:G:1179:THR:O	2:G:1181:VAL:HG23	2.19	0.42
1:A:307:GLN:HG3	1:A:352:GLN:NE2	2.33	0.42
2:E:1020:PHE:N	2:E:1021:PRO:CD	2.83	0.42
2:G:746:LEU:HA	2:G:747:PRO:HD3	1.81	0.42
1:C:283:VAL:HG12	1:C:284:GLU:H	1.84	0.42
1:C:388:ILE:O	1:C:392:VAL:HB	2.20	0.42
2:E:769:LYS:HD2	2:H:976:ASN:HA	2.02	0.42
2:G:1045:MET:O	2:G:1049:ILE:HG12	2.19	0.42
1:A:289:LEU:HD13	1:A:309:ILE:CD1	2.50	0.42
1:B:385:PHE:CZ	1:C:385:PHE:HB2	2.55	0.42
1:D:248:ILE:HG12	1:D:248:ILE:H	1.68	0.42
2:H:1059:PHE:HA	2:H:1060:PRO:HD3	1.91	0.42
1:A:297:THR:O	1:A:302:LYS:NZ	2.51	0.42
1:C:314:THR:HG23	1:C:359:GLN:OE1	2.19	0.42
1:A:370:ARG:HG3	1:A:370:ARG:HH11	1.85	0.41
1:B:350:LYS:HE3	3:B:47:HOH:O	2.20	0.41
2:E:970:MET:HA	2:H:762:LEU:HD13	2.01	0.41
2:G:932:GLN:O	2:G:936:ILE:HG12	2.20	0.41
2:F:850:PHE:HZ	2:F:873:MET:HG3	1.85	0.41
1:C:179:LEU:O	1:C:183:LEU:HG	2.20	0.41
1:D:257:LEU:O	1:D:260:LEU:HB2	2.20	0.41
1:A:287:GLN:HB3	1:A:288:PRO:HD3	2.02	0.41
1:C:418:ARG:HB3	1:C:419:PRO:HD3	2.02	0.41
1:D:309:ILE:O	1:D:313:ILE:HD13	2.21	0.41
2:E:790:GLU:HG2	2:H:962:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:881:MET:HE1	2:F:887:LEU:HD21	2.02	0.41
1:C:225:MET:HE3	1:C:225:MET:HA	2.03	0.41
2:E:877:LEU:O	2:E:881:MET:HG2	2.20	0.41
2:E:878:ILE:HD11	2:E:920:LEU:HB3	2.02	0.41
2:G:962:LEU:HD13	2:F:790:GLU:HG2	2.02	0.41
2:G:984:ILE:HD11	2:G:1105:PHE:O	2.21	0.41
2:F:746:LEU:HA	2:F:747:PRO:HD3	1.86	0.41
1:B:259:ILE:HD13	2:F:1194:ALA:HB1	2.02	0.41
2:H:954:GLU:HA	2:H:957:SER:HB3	2.03	0.41
1:A:433:VAL:CG1	1:D:410:LEU:HB2	2.51	0.41
1:B:404:ILE:HD11	1:C:426:GLU:CA	2.50	0.41
2:H:748:PHE:CD1	2:H:773:GLU:HB3	2.56	0.41
2:G:790:GLU:HG2	2:F:962:LEU:HD13	2.03	0.41
2:G:1149:LYS:HB3	2:G:1149:LYS:HE2	1.91	0.41
1:A:316:ALA:O	1:A:322:ARG:HD3	2.21	0.41
1:A:447:HIS:HD1	1:D:449:GLN:HB3	1.86	0.41
1:B:160:ARG:HD3	1:B:210:ARG:HB3	2.03	0.41
1:C:319:LEU:HD21	1:C:367:LEU:HD23	2.02	0.41
1:C:370:ARG:O	1:C:374:ILE:HG12	2.21	0.41
2:G:984:ILE:H	2:G:984:ILE:CD1	2.14	0.41
2:F:915:ARG:O	2:F:919:ARG:HB2	2.20	0.41
2:F:1088:ARG:NH1	2:F:1088:ARG:CG	2.84	0.41
2:E:845:ILE:HG21	2:G:1161:GLU:HG3	2.03	0.40
1:C:256:ALA:O	1:C:259:ILE:HG13	2.21	0.40
2:H:994:LYS:HA	2:H:1001:THR:HA	2.02	0.40
2:H:997:ASP:OD1	2:H:999:LYS:HB2	2.22	0.40
2:H:1087:LEU:HD12	2:H:1087:LEU:HA	1.95	0.40
2:G:1179:THR:HB	2:G:1180:GLY:H	1.64	0.40
2:F:1034:SER:HB3	2:F:1037:ASN:HB2	2.02	0.40
1:B:278:ALA:HB2	1:B:285:ARG:HA	2.03	0.40
1:B:341:LEU:HD22	1:B:349:MET:HE3	2.03	0.40
1:D:283:VAL:HG12	1:D:284:GLU:N	2.36	0.40
2:E:989:LYS:HE2	2:E:989:LYS:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/330 (95%)	299 (96%)	13 (4%)	1 (0%)	36	68
1	B	314/330 (95%)	296 (94%)	15 (5%)	3 (1%)	12	45
1	C	307/330 (93%)	289 (94%)	14 (5%)	4 (1%)	9	40
1	D	317/330 (96%)	296 (93%)	16 (5%)	5 (2%)	7	36
2	E	429/467 (92%)	390 (91%)	26 (6%)	13 (3%)	3	23
2	F	429/467 (92%)	387 (90%)	33 (8%)	9 (2%)	5	31
2	G	429/467 (92%)	389 (91%)	31 (7%)	9 (2%)	5	31
2	H	429/467 (92%)	384 (90%)	37 (9%)	8 (2%)	6	33
All	All	2967/3188 (93%)	2730 (92%)	185 (6%)	52 (2%)	6	34

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	C	264	GLU
1	D	447	HIS
1	D	451	ASP
2	E	975	ARG
2	E	1181	VAL
2	H	829	VAL
2	G	772	ALA
2	G	1180	GLY
2	F	772	ALA
2	F	829	VAL
2	F	1181	VAL
1	B	201	ASP
1	D	297	THR
2	E	772	ALA
2	E	787	ASP
2	H	1181	VAL

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Mol	Chain	Res	Type
2	G	829	VAL
2	G	1179	THR
1	C	295	SER
1	D	264	GLU
2	E	785	LYS
2	E	977	ALA
2	E	1062	ALA
2	E	1173	ASN
2	E	1197	ARG
2	H	972	ALA
2	G	785	LYS
2	F	972	ALA
2	F	977	ALA
1	C	297	THR
2	E	746	LEU
2	E	972	ALA
2	E	1106	VAL
2	G	746	LEU
2	G	830	LYS
2	F	746	LEU
2	F	1106	VAL
1	B	194	GLU
2	E	1174	ALA
2	H	830	LYS
2	H	884	PRO
1	B	264	GLU
2	H	746	LEU
2	F	1176	GLY
1	D	411	VAL
2	H	1106	VAL
2	H	1180	GLY
2	G	1106	VAL
2	G	884	PRO
1	C	261	PRO
2	F	884	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	287/299 (96%)	264 (92%)	23 (8%)	11	40
1	B	288/299 (96%)	270 (94%)	18 (6%)	16	48
1	C	282/299 (94%)	259 (92%)	23 (8%)	10	39
1	D	289/299 (97%)	263 (91%)	26 (9%)	9	34
2	E	391/416 (94%)	350 (90%)	41 (10%)	6	28
2	F	391/416 (94%)	367 (94%)	24 (6%)	17	49
2	G	391/416 (94%)	359 (92%)	32 (8%)	10	39
2	H	391/416 (94%)	355 (91%)	36 (9%)	8	33
All	All	2710/2860 (95%)	2487 (92%)	223 (8%)	10	39

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LYS
1	A	203	ARG
1	A	223	LYS
1	A	225	MET
1	A	235	LEU
1	A	252	LYS
1	A	260	LEU
1	A	283	VAL
1	A	299	ILE
1	A	318	GLU
1	A	329	LEU
1	A	332	LEU
1	A	334	LEU
1	A	345	GLU
1	A	367	LEU
1	A	374	ILE
1	A	391	THR
1	A	392	VAL
1	A	408	LEU
1	A	427	GLU
1	A	434	LEU
1	A	446	ARG
1	A	452	ILE
1	B	187	LYS
1	B	225	MET

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Mol	Chain	Res	Type
1	B	230	GLU
1	B	243	VAL
1	B	260	LEU
1	B	269	ARG
1	B	325	ILE
1	B	329	LEU
1	B	334	LEU
1	B	367	LEU
1	B	374	ILE
1	B	384	VAL
1	B	392	VAL
1	B	408	LEU
1	B	409	LEU
1	B	427	GLU
1	B	436	LYS
1	B	446	ARG
1	C	169	SER
1	C	187	LYS
1	C	225	MET
1	C	230	GLU
1	C	275	THR
1	C	283	VAL
1	C	290	LEU
1	C	329	LEU
1	C	332	LEU
1	C	334	LEU
1	C	367	LEU
1	C	371	LEU
1	C	377	GLU
1	C	391	THR
1	C	392	VAL
1	C	426	GLU
1	C	427	GLU
1	C	434	LEU
1	C	436	LYS
1	C	446	ARG
1	C	447	HIS
1	C	449	GLN
1	C	450	ILE
1	D	168	VAL
1	D	185	ILE
1	D	187	LYS

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Mol	Chain	Res	Type
1	D	223	LYS
1	D	225	MET
1	D	248	ILE
1	D	269	ARG
1	D	312	LEU
1	D	325	ILE
1	D	329	LEU
1	D	332	LEU
1	D	334	LEU
1	D	345	GLU
1	D	367	LEU
1	D	371	LEU
1	D	377	GLU
1	D	392	VAL
1	D	408	LEU
1	D	409	LEU
1	D	412	ARG
1	D	427	GLU
1	D	434	LEU
1	D	436	LYS
1	D	446	ARG
1	D	447	HIS
1	D	449	GLN
2	E	746	LEU
2	E	753	LYS
2	E	754	LYS
2	E	762	LEU
2	E	773	GLU
2	E	779	CYS
2	E	787	ASP
2	E	794	LEU
2	E	829	VAL
2	E	839	THR
2	E	883	GLU
2	E	916	LEU
2	E	920	LEU
2	E	936	ILE
2	E	937	LYS
2	E	950	LEU
2	E	959	LEU
2	E	976	ASN
2	E	984	ILE

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Mol	Chain	Res	Type
2	E	989	LYS
2	E	994	LYS
2	E	1002	LEU
2	E	1003	LEU
2	E	1006	LEU
2	E	1027	VAL
2	E	1059	PHE
2	E	1087	LEU
2	E	1100	GLU
2	E	1110	LYS
2	E	1111	LYS
2	E	1114	VAL
2	E	1115	GLU
2	E	1121	LEU
2	E	1125	ARG
2	E	1132	VAL
2	E	1137	LYS
2	E	1160	LEU
2	E	1169	LEU
2	E	1170	ILE
2	E	1189	LEU
2	E	1198	LYS
2	H	746	LEU
2	H	754	LYS
2	H	760	VAL
2	H	762	LEU
2	H	771	VAL
2	H	773	GLU
2	H	800	LEU
2	H	828	LYS
2	H	916	LEU
2	H	920	LEU
2	H	950	LEU
2	H	959	LEU
2	H	984	ILE
2	H	994	LYS
2	H	1000	MET
2	H	1002	LEU
2	H	1003	LEU
2	H	1016	GLU
2	H	1054	ARG
2	H	1059	PHE

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Mol	Chain	Res	Type
2	H	1065	GLU
2	H	1070	VAL
2	H	1087	LEU
2	H	1100	GLU
2	H	1103	ASP
2	H	1110	LYS
2	H	1111	LYS
2	H	1115	GLU
2	H	1116	GLU
2	H	1121	LEU
2	H	1125	ARG
2	H	1137	LYS
2	H	1160	LEU
2	H	1171	ASP
2	H	1197	ARG
2	H	1198	LYS
2	G	745	VAL
2	G	754	LYS
2	G	762	LEU
2	G	773	GLU
2	G	798	LEU
2	G	828	LYS
2	G	839	THR
2	G	849	SER
2	G	866	GLU
2	G	888	LYS
2	G	916	LEU
2	G	920	LEU
2	G	950	LEU
2	G	959	LEU
2	G	984	ILE
2	G	994	LYS
2	G	1003	LEU
2	G	1009	LEU
2	G	1054	ARG
2	G	1070	VAL
2	G	1089	MET
2	G	1100	GLU
2	G	1110	LYS
2	G	1115	GLU
2	G	1121	LEU
2	G	1125	ARG

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Mol	Chain	Res	Type
2	G	1137	LYS
2	G	1160	LEU
2	G	1179	THR
2	G	1187	GLU
2	G	1189	LEU
2	G	1197	ARG
2	F	750	LEU
2	F	754	LYS
2	F	762	LEU
2	F	773	GLU
2	F	788	ARG
2	F	839	THR
2	F	866	GLU
2	F	950	LEU
2	F	959	LEU
2	F	989	LYS
2	F	994	LYS
2	F	1003	LEU
2	F	1016	GLU
2	F	1059	PHE
2	F	1089	MET
2	F	1100	GLU
2	F	1114	VAL
2	F	1115	GLU
2	F	1121	LEU
2	F	1125	ARG
2	F	1139	ARG
2	F	1160	LEU
2	F	1170	ILE
2	F	1198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	190	HIS
1	A	206	HIS
1	A	359	GLN
1	B	190	HIS
1	B	199	ASN
1	B	204	ASN
1	B	205	GLN

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Mol	Chain	Res	Type
1	B	359	GLN
1	B	447	HIS
1	C	141	GLN
1	C	206	HIS
1	C	336	GLN
1	C	431	GLN
1	C	449	GLN
1	D	141	GLN
1	D	190	HIS
1	D	217	ASN
1	D	339	GLN
1	D	447	HIS
2	E	766	ASN
2	E	791	ASN
2	E	792	ASN
2	E	859	ASN
2	E	876	ASN
2	E	880	GLN
2	E	935	ASN
2	E	1083	GLN
2	E	1164	GLN
2	E	1168	GLN
2	H	791	ASN
2	H	841	GLN
2	H	859	ASN
2	H	880	GLN
2	H	998	GLN
2	H	1014	HIS
2	H	1057	GLN
2	H	1091	HIS
2	G	841	GLN
2	G	875	GLN
2	G	876	ASN
2	G	880	GLN
2	G	886	GLN
2	G	935	ASN
2	G	968	ASN
2	G	998	GLN
2	G	1048	GLN
2	G	1057	GLN
2	G	1093	ASN
2	G	1122	HIS

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Mol	Chain	Res	Type
2	G	1168	GLN
2	F	842	ASN
2	F	859	ASN
2	F	865	ASN
2	F	875	GLN
2	F	876	ASN
2	F	880	GLN
2	F	935	ASN
2	F	1012	ASN
2	F	1085	ASN
2	F	1093	ASN
2	F	1168	GLN
2	F	1173	ASN

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 [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	317/330 (96%)	-0.35	4 (1%) 75 55	15, 75, 117, 149	2 (0%)
1	B	318/330 (96%)	-0.36	2 (0%) 85 73	22, 79, 131, 157	2 (0%)
1	C	311/330 (94%)	-0.34	2 (0%) 85 73	15, 80, 129, 213	2 (0%)
1	D	319/330 (96%)	0.10	6 (1%) 66 46	16, 112, 166, 198	2 (0%)
2	E	433/467 (92%)	-0.13	2 (0%) 87 76	47, 94, 144, 177	0
2	F	433/467 (92%)	0.28	9 (2%) 63 43	61, 133, 211, 256	0
2	G	433/467 (92%)	0.29	8 (1%) 67 48	68, 127, 172, 209	0
2	H	433/467 (92%)	0.07	3 (0%) 84 69	40, 110, 166, 200	0
All	All	2997/3188 (94%)	-0.03	36 (1%) 76 58	15, 102, 173, 256	8 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	HIS	5.3
1	D	415	TYR	5.2
2	F	787	ASP	3.4
1	A	452	ILE	3.3
2	F	1198	LYS	3.2
1	C	411	VAL	3.1
1	B	411	VAL	3.1
1	A	411	VAL	3.0
2	F	806	THR	2.7
2	H	789	PHE	2.6
2	F	829	VAL	2.6
2	G	1070	VAL	2.6
1	D	211	CYS	2.5
2	G	785	LYS	2.5
2	F	906	PHE	2.5
2	G	806	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	170	TRP	2.4
2	F	832	LEU	2.4
2	E	748	PHE	2.4
1	A	200	TYR	2.3
2	G	893	LEU	2.3
1	B	217	ASN	2.3
2	H	787	ASP	2.3
2	H	792	ASN	2.3
2	G	1166	ARG	2.2
2	G	777	GLN	2.2
1	D	428	CYS	2.2
2	G	1053	GLU	2.2
2	F	789	PHE	2.2
2	F	867	ALA	2.1
1	D	452	ILE	2.1
2	G	1170	ILE	2.1
1	A	334	LEU	2.1
2	E	787	ASP	2.1
1	D	445	CYS	2.1
2	F	804	ALA	2.1

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.