



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:58 pm BST

PDB ID : 3O4X
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

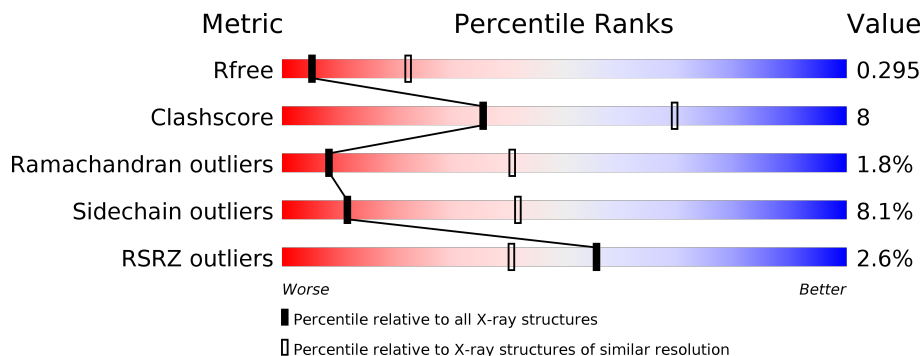
1 Overall quality at a glance

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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	
1	B	330	
1	C	330	
1	D	330	
2	E	467	
2	F	467	

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Mol	Chain	Length	Quality of chain
2	G	467	 <p>3% 70% 19% • 7%</p>
2	H	467	 <p>2% 72% 16% • 7%</p>

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

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
			Total	C	N	O	S			
2	E	433	3525	2230	602	672	21	0	0	0
2	H	433	3525	2230	602	672	21	0	0	0
2	G	433	3525	2230	602	672	21	0	0	0
2	F	433	3525	2230	602	672	21	0	0	0

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

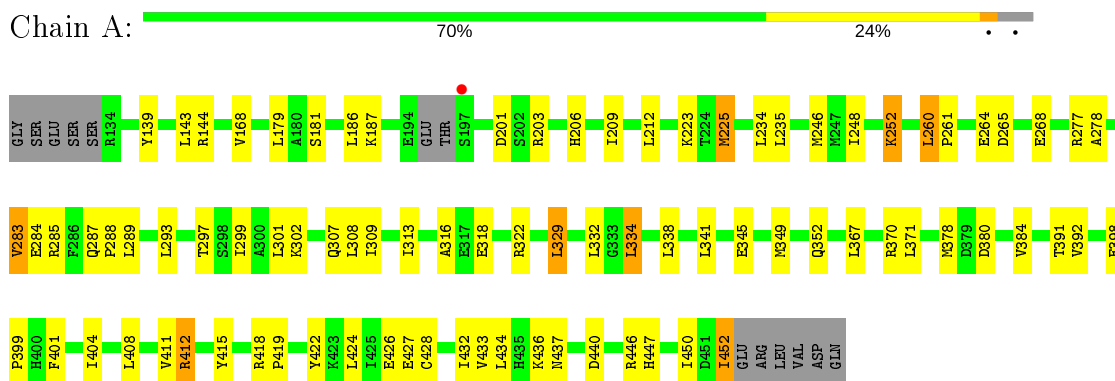
- Molecule 3 is water.

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

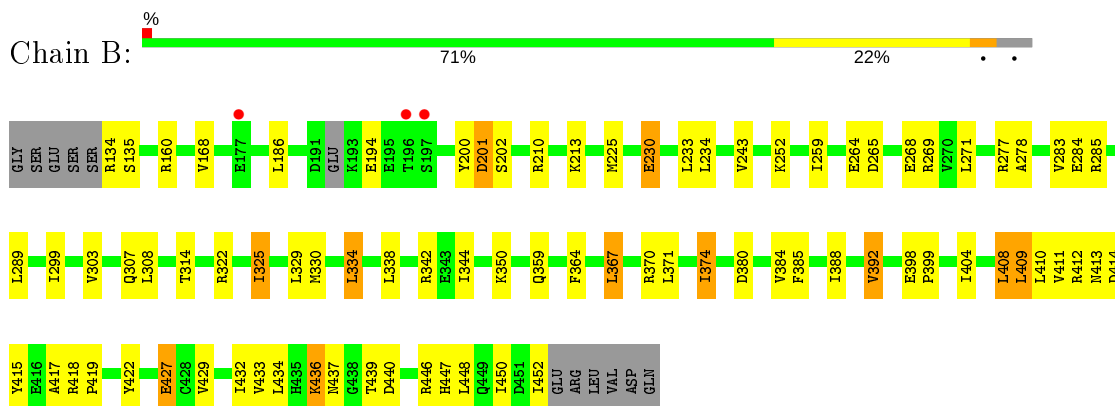
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

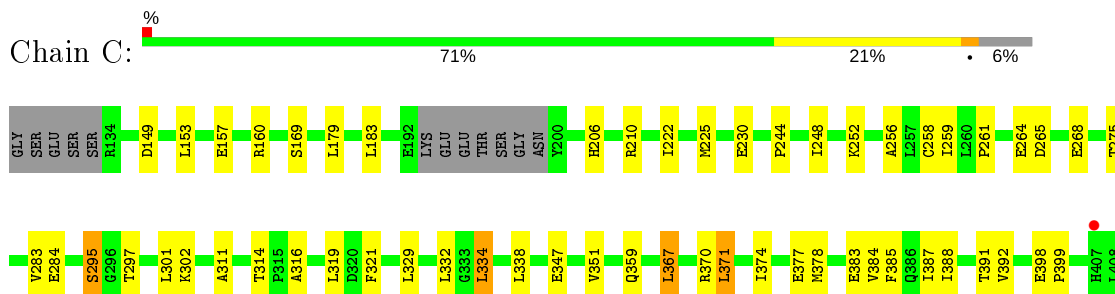
- Molecule 1: Protein diaphanous homolog 1

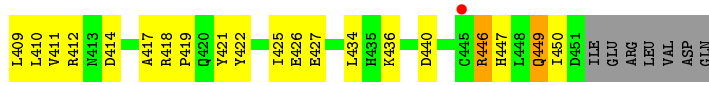


- Molecule 1: Protein diaphanous homolog 1

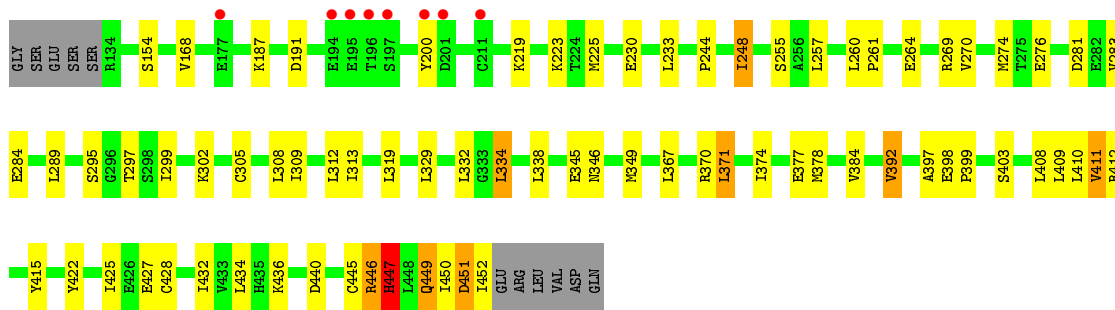
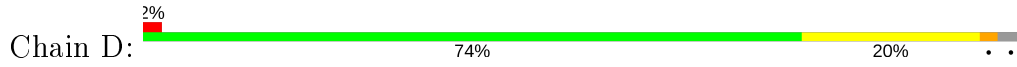


- Molecule 1: Protein diaphanous homolog 1

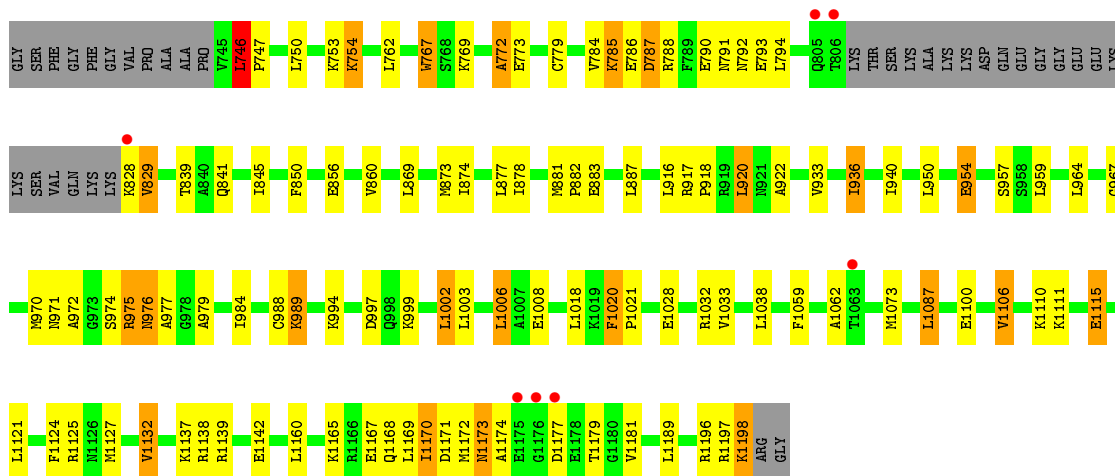




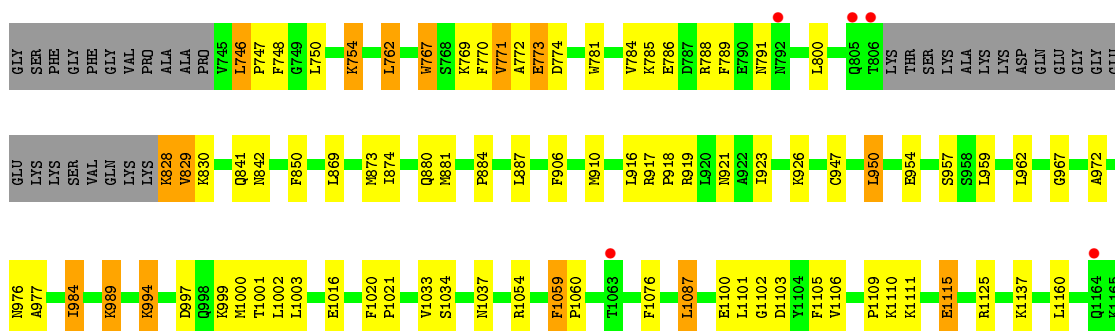
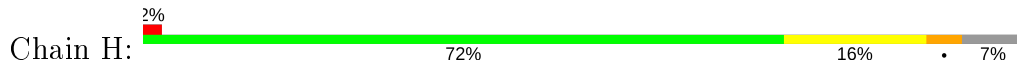
• Molecule 1: Protein diaphanous homolog 1

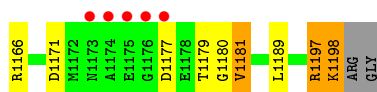


• Molecule 2: Protein diaphanous homolog 1

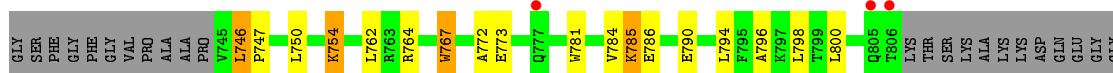


• Molecule 2: Protein diaphanous homolog 1

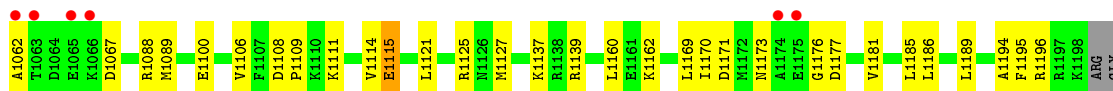
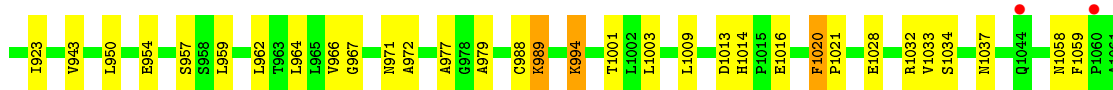
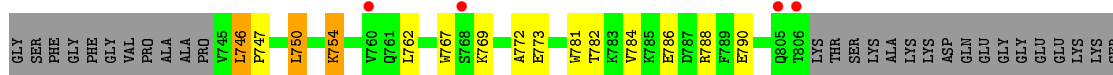
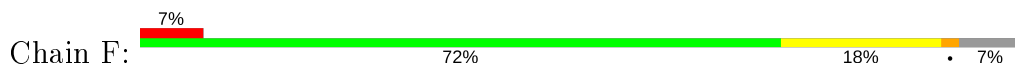




• Molecule 2: Protein diaphanous homolog 1



• 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) 99.1 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.36	0/2588	0.58	0/3483
1	B	0.37	0/2595	0.56	0/3493
1	C	0.37	0/2544	0.55	1/3425 (0.0%)
1	D	0.36	0/2605	0.55	1/3508 (0.0%)
2	E	0.37	0/3580	0.55	0/4799
2	F	0.36	0/3580	0.53	0/4799
2	G	0.36	0/3580	0.53	0/4799
2	H	0.38	0/3580	0.53	0/4799
All	All	0.37	0/24652	0.55	2/33105 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	LEU	CA-CB-CG	6.41	130.03	115.30
1	D	371	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2552	0	2563	59	0
1	B	2559	0	2570	73	0
1	C	2508	0	2519	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2568	0	2577	47	0
2	E	3525	0	3552	65	0
2	F	3525	0	3552	57	0
2	G	3525	0	3552	67	0
2	H	3525	0	3552	52	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	396	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 (396) 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	1.34	1.09
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
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:HH11	1:B:446:ARG:HG3	1.42	0.83
2:G:750:LEU:HB2	2:G:785:LYS:HD3	1.59	0.82
1:D:411:VAL:O	1:D:411:VAL:HG23	1.78	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:784:VAL:C	2:E:786:GLU:H	1.91	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
1:B:388:ILE:HG12	1:C:409:LEU:HD12	1.70	0.71
1:B:411:VAL:O	1:B:411:VAL:HG23	1.90	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: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
2:G:784:VAL:C	2:G:786:GLU:H	1.94	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:H:1033:VAL:HG12	2:H:1034:SER:H	1.61	0.65
1:D:411:VAL:O	1:D:411:VAL:CG2	2.45	0.65
1:B:427:GLU:HG2	1:B:452:ILE:HG22	1.76	0.65
1:B:388:ILE:CG1	1:C:409:LEU:CD1	2.75	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:1002:LEU:HD22	2:E:1006:LEU:CD1	2.28	0.64
1:B:200:TYR:C	1:B:202:SER:H	1.98	0.64
2:F:1033:VAL:O	2:F:1115:GLU:HG2	1.98	0.64
1:A:411:VAL:O	1:A:411:VAL:HG23	1.97	0.63
1:B:436:LYS:O	1:B:437:ASN:HB2	1.98	0.63
2:E:1033:VAL:O	2:E:1115:GLU:CG	2.46	0.63
1:D:168:VAL:HG21	2:H:1177:ASP:HB3	1.79	0.63
1:A:168:VAL:HG11	2:E:1177:ASP:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:856:GLU:O	2:G:860:VAL:HG23	1.99	0.63
2:G:976:ASN:HA	2:F:769:LYS:HD2	1.82	0.62
1:C:411:VAL:O	1:C:411:VAL:HG23	1.99	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
2:F:988:CYS:HA	2:F:1127:MET:CE	2.30	0.61
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:HH11	1:B:370:ARG:HG3	1.66	0.61
2:E:784:VAL:C	2:E:786:GLU:N	2.54	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:O	1:A:411:VAL:CG2	2.49	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
2:F:1062:ALA:HB1	2:F:1067:ASP:HB3	1.84	0.59
1:B:200:TYR:C	1:B:202:SER:N	2.56	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:E:786:GLU:C	2:E:788:ARG:H	2.07	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: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
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:N	2:G:754:LYS:HE2	2.13	0.57
1:C:398:GLU:HB3	1:C:399:PRO:HD3	1.85	0.57
2:G:954:GLU:HA	2:G:957:SER:HB3	1.87	0.56
2:H:917:ARG:HB3	2:H:918:PRO:HD3	1.87	0.56
1:C:383:GLU:O	1:C:387:ILE:HD13	2.05	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:881:MET:HE1	2:H:887:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:915:ARG:HH22	2:F:1058:ASN:HB3	1.71	0.55
2:G:1158:GLU:HB3	2:G:1198:LYS:HE2	1.89	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
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:B:411:VAL:O	1:B:411:VAL:CG2	2.54	0.54
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:CG	1:B:446:ARG:HH11	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:D:302:LYS:HB3	1:D:349:MET:HE3	1.90	0.54
1:A:428:CYS:O	1:A:432:ILE:HD13	2.08	0.54
1:C:153:LEU:O	1:C:157:GLU:HB2	2.08	0.54
1:B:388:ILE:HG13	1:C:409:LEU:HD11	1.88	0.54
2:F:919:ARG:O	2:F:923:ILE:HG12	2.07	0.54
2:F:988:CYS:HA	2:F:1127:MET:HE1	1.89	0.54
2:F:830:LYS:HD3	2:F:901:ALA:HA	1.90	0.54
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: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
1:B:392:VAL:HG13	1:B:398:GLU:HA	1.90	0.53
1:A:432:ILE:HG21	1:D:425:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1028:GLU:HG2	2:E:1032:ARG:HH21	1.75	0.52
2:E:936:ILE:O	2:E:940:ILE:HG12	2.09	0.52
2:G:832:LEU:HD21	2:G:840:ALA:CB	2.40	0.52
2:H:1034:SER:HB3	2:H:1037:ASN:HB2	1.91	0.52
1:B:271:LEU:HD21	1:B:325:ILE:HD11	1.92	0.52
1:B:303:VAL:O	1:B:307:GLN:HB2	2.10	0.51
1:A:419:PRO:HA	1:D:397:ALA:HB2	1.91	0.51
1:A:168:VAL:HG22	2:E:1179:THR:HG23	1.92	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
2:G:784:VAL:C	2:G:786:GLU:N	2.63	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:C:347:GLU:O	1:C:351:VAL:HG23	2.11	0.51
1:B:371:LEU:HB2	1:C:410:LEU:HD11	1.93	0.51
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:N	2:G:984:ILE:HD12	2.24	0.50
2:H:950:LEU:CD1	2:H:1105:PHE:HE1	2.24	0.50
2:F:784:VAL:C	2:F:786:GLU:H	2.14	0.50
1:B:168:VAL:HG11	2:F:1177:ASP:HB3	1.93	0.50
2:F:964:LEU:HD11	2:F:979:ALA:O	2.11	0.50
1:D:261:PRO:HG3	2:H:1166:ARG:HG2	1.93	0.50
2:H:881:MET:CE	2:H:887:LEU:HD11	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1124:PHE:HA	2:E:1127:MET:HE2	1.94	0.49
2:E:850:PHE:HZ	2:E:873:MET:HG3	1.77	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:G:764:ARG:HD2	2:F:971:ASN:HA	1.95	0.49
2:H:926:LYS:HA	2:H:1076:PHE:CZ	2.48	0.49
1:B:299:ILE:HD11	1:B:344:ILE:HG23	1.95	0.48
2:E:793:GLU:HA	2:E:793:GLU:OE1	2.13	0.48
2:H:784:VAL:C	2:H:786:GLU:H	2.16	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:E:922:ALA:HB1	2:E:1073:MET:HE2	1.94	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:E:1171:ASP:C	2:E:1173:ASN:H	2.17	0.48
2:F:754:LYS:N	2:F:754:LYS:HE2	2.23	0.48
2:F:943:VAL:HG11	2:F:1114:VAL:HG11	1.96	0.48
2:G:1179:THR:O	2:G:1181:VAL:N	2.46	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
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:F:988:CYS:HA	2:F:1127:MET:HE2	1.95	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
1:A:302:LYS:HB3	1:A:349:MET:HE1	1.96	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:F:754:LYS:H	2:F:754:LYS:CE	2.23	0.47
2:H:841:GLN:HE22	2:F:1196:ARG:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HE	1:A:181:SER:HB3	1.78	0.47
1:B:404:ILE:HD11	1:C:426:GLU:N	2.29	0.47
1:B:314:THR:HG21	2:F:1195:PHE:HB3	1.96	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:D:302:LYS:HB3	1:D:349:MET:CE	2.45	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:C:222:ILE:HG21	2:G:1172:MET:HE3	1.96	0.46
1:B:433:VAL:CG1	1:C:410:LEU:HB3	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: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
2:G:1048:GLN:HA	2:G:1051:ASP:HB2	1.98	0.46
2:G:847:LEU:HD22	2:G:854:TYR:HE1	1.79	0.46
2:H:784:VAL:C	2:H:786:GLU:N	2.68	0.46
2:E:1008:GLU:HG3	2:E:1139:ARG:HH21	1.81	0.46
2:E:933:VAL:HG13	2:E:1087:LEU:HD21	1.98	0.46
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:1198:LYS:HE2	2:G:879:LYS:NZ	2.30	0.46
2:E:917:ARG:HB3	2:E:918:PRO:HD3	1.98	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:440:ASP:CG	1:C:412:ARG:HH21	2.20	0.45
2:F:750:LEU:HD22	2:F:782:THR:HG23	1.98	0.45
2:H:754:LYS:H	2:H:754:LYS:HE2	1.81	0.45
1:B:415:TYR:CG	2:H:989:LYS:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:1169:LEU:HD11	2:F:1194:ALA:HA	1.99	0.45
2:H:842:ASN:HB3	2:H:880:GLN:HE22	1.81	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:F:846:PHE:HE1	2:F:876:ASN:HB3	1.80	0.45
2:G:1020:PHE:N	2:G:1021:PRO:CD	2.80	0.45
2:E:841:GLN:HG3	2:G:1168:GLN:NE2	2.30	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:E:746:LEU:HA	2:E:747:PRO:HD3	1.67	0.45
1:A:329:LEU:HB3	1:A:334:LEU:HD12	1.99	0.44
2:F:1088:ARG:NH1	2:F:1088:ARG:HG2	2.28	0.44
2:H:786:GLU:HB3	2:H:789:PHE:HB2	1.99	0.44
1:B:404:ILE:HD11	1:C:426:GLU:HA	1.99	0.44
2:F:1088:ARG:CG	2:F:1088:ARG:HH11	2.26	0.44
2:G:767:TRP:HH2	2:F:967:GLY:HA3	1.83	0.44
2:G:966:VAL:O	2:G:970:MET:HG3	2.18	0.44
2:H:747:PRO:HB3	2:H:772:ALA:HB1	2.00	0.44
2:G:1034:SER:HB3	2:G:1037:ASN:HB2	2.00	0.44
2:H:771:VAL:HG12	2:H:774:ASP:OD2	2.18	0.44
2:H:750:LEU:HB2	2:H:785:LYS:HD3	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:295:SER:HA	1:D:302:LYS:CE	2.48	0.44
1:D:276:GLU:HA	2:G:975:ARG:HD3	2.00	0.44
1:B:299:ILE:HD11	1:B:344:ILE:HG21	1.99	0.44
1:A:261:PRO:HB3	2:E:1167:GLU:HG2	2.00	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:C:160:ARG:CD	1:C:210:ARG:HB3	2.48	0.43
1:B:134:ARG:HB3	1:B:135:SER:H	1.58	0.43
2:E:856:GLU:O	2:E:860:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.66	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:C:411:VAL:O	1:C:411:VAL:CG2	2.63	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
2:G:1111:LYS:HD3	2:G:1111:LYS:HA	1.82	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
2:E:767:TRP:CH2	2:H:967:GLY:HA3	2.54	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:297:THR:O	1:A:302:LYS:NZ	2.51	0.42
2:E:974:SER:O	2:E:975:ARG:C	2.56	0.42
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
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.93	0.42
1:C:258:CYS:HB3	1:C:311:ALA:O	2.19	0.42
1:A:426:GLU:HG3	1:D:403:SER:HB3	2.00	0.42
2:F:1108:ASP:HA	2:F:1109:PRO:HD3	1.90	0.42
2:F:1127:MET:HB2	2:F:1127:MET:HE3	1.94	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:H	1:D:248:ILE:HG12	1.68	0.42
2:H:1059:PHE:HA	2:H:1060:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:THR:HG23	1:C:359:GLN:OE1	2.19	0.42
1:A:370:ARG:HH11	1:A:370:ARG:HG3	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:F:850:PHE:HZ	2:F:873:MET:HG3	1.85	0.41
2:G:932:GLN:O	2:G:936:ILE:HG12	2.20	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
2:E:786:GLU:C	2:E:788:ARG:N	2.72	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
2:E:877:LEU:O	2:E:881:MET:HG2	2.20	0.41
2:E:881:MET:HE3	2:E:882:PRO:HD2	2.03	0.41
2:E:878:ILE:HD11	2:E:920:LEU:HB3	2.02	0.41
2:F:746:LEU:HA	2:F:747:PRO:HD3	1.86	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
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:B:404:ILE:HD11	1:C:426:GLU:CA	2.50	0.41
1:A:433:VAL:CG1	1:D:410:LEU:HB2	2.51	0.41
2:G:790:GLU:HG2	2:F:962:LEU:HD13	2.03	0.41
2:H:748:PHE:CD1	2:H:773:GLU:HB3	2.56	0.41
2:G:1149:LYS:HE2	2:G:1149:LYS:HB3	1.91	0.41
1:A:316:ALA:O	1:A:322:ARG:HD3	2.21	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:F:915:ARG:O	2:F:919:ARG:HB2	2.20	0.41
1:B:160:ARG:HD3	1:B:210:ARG:HB3	2.03	0.41
1:A:447:HIS:HD1	1:D:449:GLN:HB3	1.86	0.41
2:G:984:ILE:CD1	2:G:984:ILE:H	2.14	0.41
2:F:1088:ARG:NH1	2:F:1088:ARG:CG	2.84	0.41
1:C:410:LEU:O	1:C:411:VAL:C	2.59	0.40
2:E:845:ILE:HG21	2:G:1161:GLU:HG3	2.03	0.40
1:A:179:LEU:HD21	1:A:225:MET:HE3	2.03	0.40
1:C:256:ALA:O	1:C:259:ILE:HG13	2.21	0.40
2:F:1034:SER:HB3	2:F:1037:ASN:HB2	2.02	0.40
2:G:1179:THR:HB	2:G:1180:GLY:H	1.64	0.40
2:H:994:LYS:HA	2:H:1001:THR:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1087:LEU:HD12	2:H:1087:LEU:HA	1.95	0.40
2:H:997:ASP:OD1	2:H:999:LYS:HB2	2.22	0.40
1:B:278:ALA:HB2	1:B:285:ARG:HA	2.03	0.40
1:D:283:VAL:HG12	1:D:284:GLU:N	2.36	0.40
2:H:1197:ARG:O	2:H:1198:LYS:C	2.60	0.40
2:E:989:LYS:HE2	2:E:989:LYS:HB3	1.91	0.40
2:F:1171:ASP:C	2:F:1173:ASN:H	2.25	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	313/330 (95%)	299 (96%)	13 (4%)	1 (0%)	41 74
1	B	314/330 (95%)	296 (94%)	15 (5%)	3 (1%)	15 54
1	C	307/330 (93%)	289 (94%)	14 (5%)	4 (1%)	12 47
1	D	317/330 (96%)	296 (93%)	16 (5%)	5 (2%)	9 43
2	E	429/467 (92%)	390 (91%)	26 (6%)	13 (3%)	4 28
2	F	429/467 (92%)	387 (90%)	33 (8%)	9 (2%)	7 37
2	G	429/467 (92%)	389 (91%)	31 (7%)	9 (2%)	7 37
2	H	429/467 (92%)	384 (90%)	37 (9%)	8 (2%)	8 39
All	All	2967/3188 (93%)	2730 (92%)	185 (6%)	52 (2%)	8 41

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	C	264	GLU
1	D	447	HIS

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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%)	12	42
1	B	288/299 (96%)	270 (94%)	18 (6%)	18	52
1	C	282/299 (94%)	264 (94%)	18 (6%)	17	52
1	D	289/299 (97%)	262 (91%)	27 (9%)	9	33
2	E	391/416 (94%)	351 (90%)	40 (10%)	7	29
2	F	391/416 (94%)	363 (93%)	28 (7%)	14	47
2	G	391/416 (94%)	358 (92%)	33 (8%)	11	39
2	H	391/416 (94%)	358 (92%)	33 (8%)	11	39
All	All	2710/2860 (95%)	2490 (92%)	220 (8%)	11	42

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LYS
1	A	201	ASP
1	A	203	ARG
1	A	223	LYS
1	A	225	MET
1	A	235	LEU
1	A	252	LYS
1	A	260	LEU

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Mol	Chain	Res	Type
1	A	277	ARG
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	391	THR
1	A	412	ARG
1	A	427	GLU
1	A	434	LEU
1	A	446	ARG
1	A	452	ILE
1	B	201	ASP
1	B	213	LYS
1	B	225	MET
1	B	230	GLU
1	B	243	VAL
1	B	269	ARG
1	B	277	ARG
1	B	322	ARG
1	B	325	ILE
1	B	329	LEU
1	B	334	LEU
1	B	367	LEU
1	B	374	ILE
1	B	392	VAL
1	B	408	LEU
1	B	409	LEU
1	B	427	GLU
1	B	436	LYS
1	C	149	ASP
1	C	169	SER
1	C	225	MET
1	C	230	GLU
1	C	275	THR
1	C	329	LEU
1	C	332	LEU
1	C	334	LEU
1	C	367	LEU

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Mol	Chain	Res	Type
1	C	377	GLU
1	C	391	THR
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	154	SER
1	D	187	LYS
1	D	191	ASP
1	D	200	TYR
1	D	223	LYS
1	D	225	MET
1	D	248	ILE
1	D	269	ARG
1	D	281	ASP
1	D	312	LEU
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	427	GLU
1	D	428	CYS
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	767	TRP
2	E	773	GLU

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Mol	Chain	Res	Type
2	E	779	CYS
2	E	787	ASP
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	950	LEU
2	E	954	GLU
2	E	959	LEU
2	E	976	ASN
2	E	984	ILE
2	E	989	LYS
2	E	994	LYS
2	E	1002	LEU
2	E	1003	LEU
2	E	1006	LEU
2	E	1020	PHE
2	E	1059	PHE
2	E	1087	LEU
2	E	1100	GLU
2	E	1110	LYS
2	E	1111	LYS
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	762	LEU
2	H	767	TRP
2	H	771	VAL
2	H	773	GLU
2	H	800	LEU
2	H	828	LYS

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Mol	Chain	Res	Type
2	H	916	LEU
2	H	921	ASN
2	H	950	LEU
2	H	959	LEU
2	H	984	ILE
2	H	989	LYS
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
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	1125	ARG
2	H	1137	LYS
2	H	1160	LEU
2	H	1171	ASP
2	H	1197	ARG
2	H	1198	LYS
2	G	754	LYS
2	G	762	LEU
2	G	767	TRP
2	G	773	GLU
2	G	828	LYS
2	G	839	THR
2	G	849	SER
2	G	850	PHE
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	989	LYS
2	G	994	LYS
2	G	1003	LEU

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Mol	Chain	Res	Type
2	G	1009	LEU
2	G	1054	ARG
2	G	1059	PHE
2	G	1100	GLU
2	G	1110	LYS
2	G	1111	LYS
2	G	1115	GLU
2	G	1121	LEU
2	G	1125	ARG
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	G	1198	LYS
2	F	750	LEU
2	F	754	LYS
2	F	762	LEU
2	F	767	TRP
2	F	773	GLU
2	F	788	ARG
2	F	839	THR
2	F	850	PHE
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	1013	ASP
2	F	1016	GLU
2	F	1020	PHE
2	F	1059	PHE
2	F	1089	MET
2	F	1100	GLU
2	F	1111	LYS
2	F	1115	GLU
2	F	1121	LEU
2	F	1125	ARG
2	F	1137	LYS
2	F	1139	ARG

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Mol	Chain	Res	Type
2	F	1160	LEU
2	F	1170	ILE

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

Mol	Chain	Res	Type
1	A	206	HIS
1	A	359	GLN
1	B	190	HIS
1	B	199	ASN
1	B	205	GLN
1	B	359	GLN
1	B	447	HIS
1	B	449	GLN
1	C	206	HIS
1	C	449	GLN
1	D	190	HIS
1	D	339	GLN
1	D	447	HIS
2	E	791	ASN
2	E	792	ASN
2	E	859	ASN
2	E	880	GLN
2	E	935	ASN
2	E	998	GLN
2	E	1168	GLN
2	H	791	ASN
2	H	841	GLN
2	H	859	ASN
2	H	880	GLN
2	H	976	ASN
2	H	1168	GLN
2	G	841	GLN
2	G	859	ASN
2	G	876	ASN
2	G	880	GLN
2	G	976	ASN
2	G	998	GLN
2	G	1039	GLN
2	G	1122	HIS
2	G	1168	GLN
2	F	841	GLN

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Mol	Chain	Res	Type
2	F	859	ASN
2	F	876	ASN
2	F	880	GLN
2	F	932	GLN
2	F	1014	HIS
2	F	1085	ASN
2	F	1168	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 carbohydrates 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%)	-0.45	1 (0%) 94 92	30, 75, 117, 149	2 (0%)
1	B	318/330 (96%)	-0.45	3 (0%) 84 75	38, 79, 131, 157	2 (0%)
1	C	311/330 (94%)	-0.45	2 (0%) 89 83	30, 80, 129, 213	2 (0%)
1	D	319/330 (96%)	-0.14	8 (2%) 57 43	31, 112, 166, 198	2 (0%)
2	E	433/467 (92%)	-0.23	7 (1%) 72 59	47, 94, 144, 177	0
2	F	433/467 (92%)	0.22	32 (7%) 14 8	61, 133, 211, 256	0
2	G	433/467 (92%)	0.08	14 (3%) 47 31	68, 127, 172, 209	0
2	H	433/467 (92%)	-0.08	10 (2%) 60 47	40, 110, 166, 200	0
All	All	2997/3188 (94%)	-0.16	77 (2%) 56 40	30, 102, 173, 256	8 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	899	ASP	7.9
2	F	806	THR	6.5
2	F	831	GLU	6.4
2	F	832	LEU	4.8
2	H	1176	GLY	4.3
2	H	1174	ALA	4.2
2	H	1173	ASN	4.2
2	G	805	GLN	4.1
1	D	196	THR	4.1
2	F	1065	GLU	4.0
2	H	1175	GLU	4.0
2	F	867	ALA	3.9
2	E	806	THR	3.9
2	F	896	GLU	3.8
2	G	806	THR	3.7
2	F	1174	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	844	SER	3.5
2	F	1060	PRO	3.4
2	F	894	LYS	3.3
2	G	895	GLU	3.3
2	F	885	GLU	3.2
2	G	828	LYS	3.2
1	B	197	SER	3.2
2	E	805	GLN	3.2
1	D	197	SER	3.1
2	F	895	GLU	3.1
2	F	838	LYS	3.0
2	F	893	LEU	3.0
1	B	196	THR	3.0
2	F	1063	THR	3.0
2	E	828	LYS	2.9
2	G	1074	THR	2.8
2	G	829	VAL	2.8
2	F	892	GLU	2.8
2	H	806	THR	2.8
2	G	777	GLN	2.7
1	C	407	HIS	2.7
2	F	805	GLN	2.7
1	D	201	ASP	2.6
2	H	805	GLN	2.6
1	D	200	TYR	2.6
2	F	1044	GLN	2.6
1	B	177	GLU	2.6
2	F	912	THR	2.5
2	G	1063	THR	2.5
2	G	1175	GLU	2.5
2	H	792	ASN	2.5
2	H	1177	ASP	2.5
1	D	194	GLU	2.4
2	F	760	VAL	2.4
2	H	1063	THR	2.4
2	G	1065	GLU	2.4
2	F	903	SER	2.4
2	F	828	LYS	2.4
2	F	829	VAL	2.3
2	F	1066	LYS	2.3
1	C	445	CYS	2.3
2	F	853	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	914	PRO	2.2
2	E	1177	ASP	2.2
2	E	1063	THR	2.2
2	H	1164	GLN	2.2
2	F	768	SER	2.2
1	D	195	GLU	2.2
2	G	1057	GLN	2.1
2	E	1176	GLY	2.1
1	A	197	SER	2.1
2	G	1092	SER	2.1
2	E	1175	GLU	2.1
2	G	1177	ASP	2.1
1	D	177	GLU	2.1
2	F	1062	ALA	2.1
2	F	1175	GLU	2.0
1	D	211	CYS	2.0
2	F	834	VAL	2.0
2	F	879	LYS	2.0
2	G	1082	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.