Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 01:50 PM EDT

PDB ID	:	4M1C
Title	:	Crystal Structure Analysis of Fab-Bound Human Insulin Degrading Enzyme (IDE) in Complex with Amyloid-Beta (1-40)
Authors	:	McCord, L.M.; Liang, W.; Farcasanu, M.; Scherpelz, K.; Meredith, S.C.; Koide, S.; Tang, W.J.
Deposited on	:	2013-08-02
Resolution	:	3.50 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:

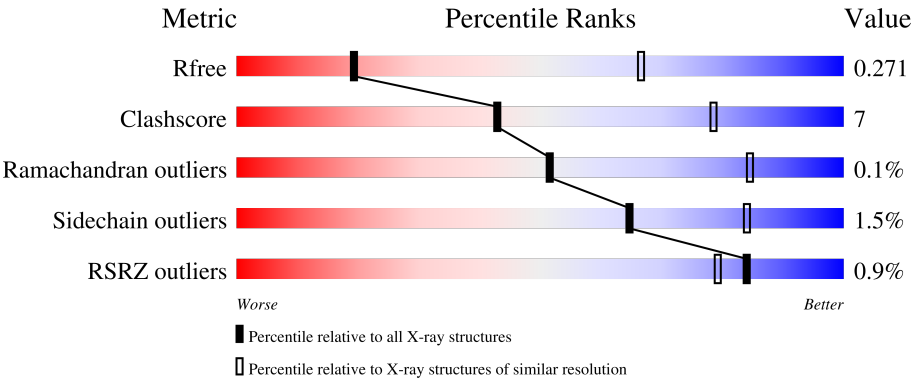
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	990	81% 16%
1	B	990	80% 16%
2	C	263	60% 17% 22%
2	E	263	56% 21% 22%
3	D	239	5% 63% 10% 27%

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Mol	Chain	Length	Quality of chain
3	F	239	
4	G	40	
4	H	40	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21509 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	957	Total	C	N	O	S	0	0	0
			7779	5014	1309	1434	22			
1	B	952	Total	C	N	O	S	0	0	0
			7745	4992	1301	1430	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called Fab-bound IDE, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	205	Total	C	N	O	S	0	0	0
			1562	999	256	300	7			
2	E	206	Total	C	N	O	S	0	0	0
			1567	999	258	303	7			

- Molecule 3 is a protein called Fab-bound IDE, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	175	Total	C	N	O	S	0	0	0
			1339	846	220	269	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	184	Total	C	N	O	S	0	0	0
			1409	883	237	284	5			

- Molecule 4 is a protein called Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	10	Total	C	N	O	0	0	0
			84	59	11	14			
4	H	3	Total	C	N	O	0	0	0
			22	12	3	7			

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

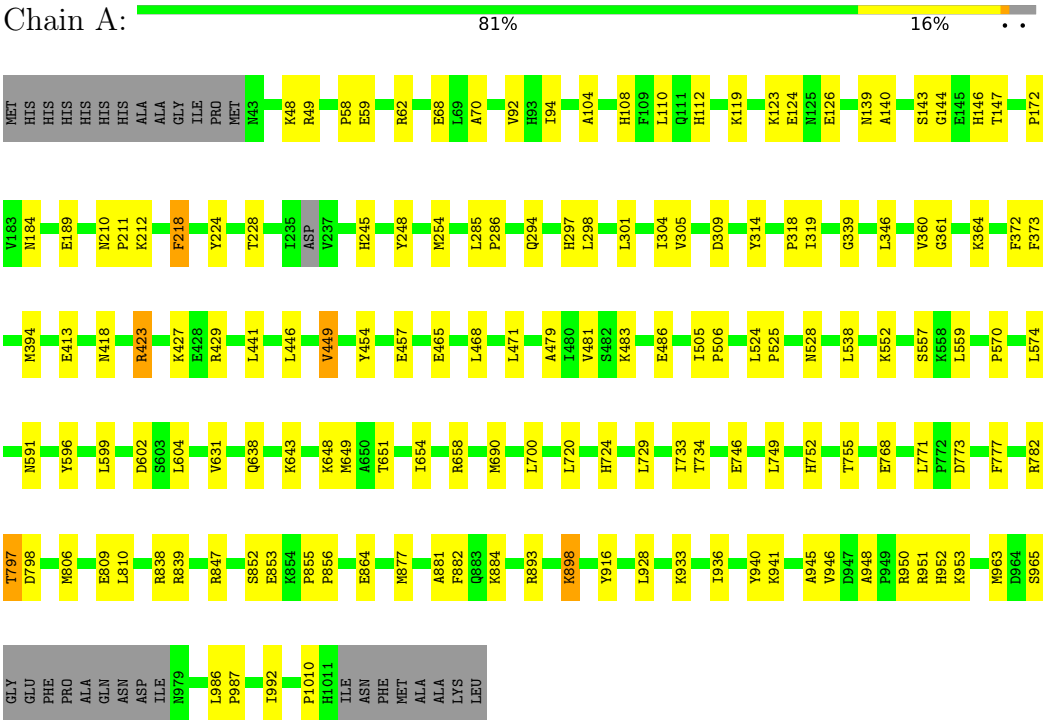
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

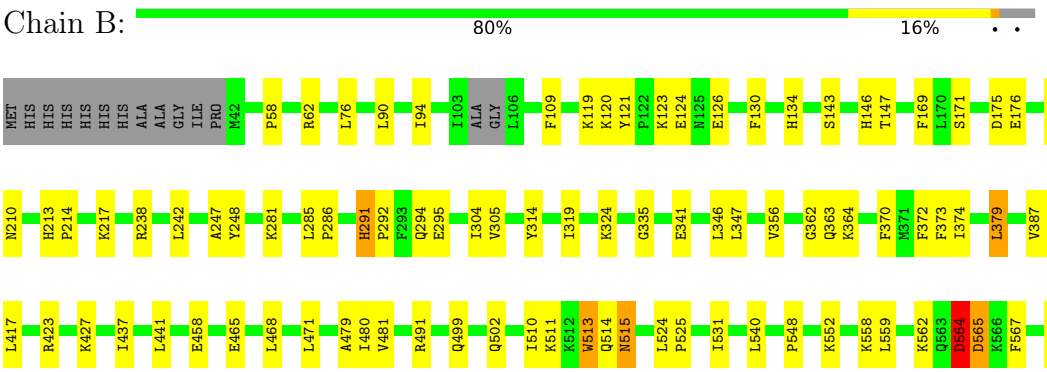
• Molecule 1: Insulin-degrading enzyme

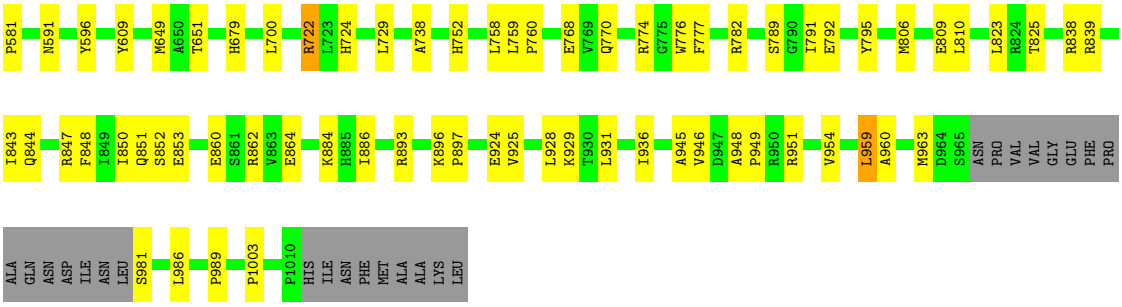
Chain A:



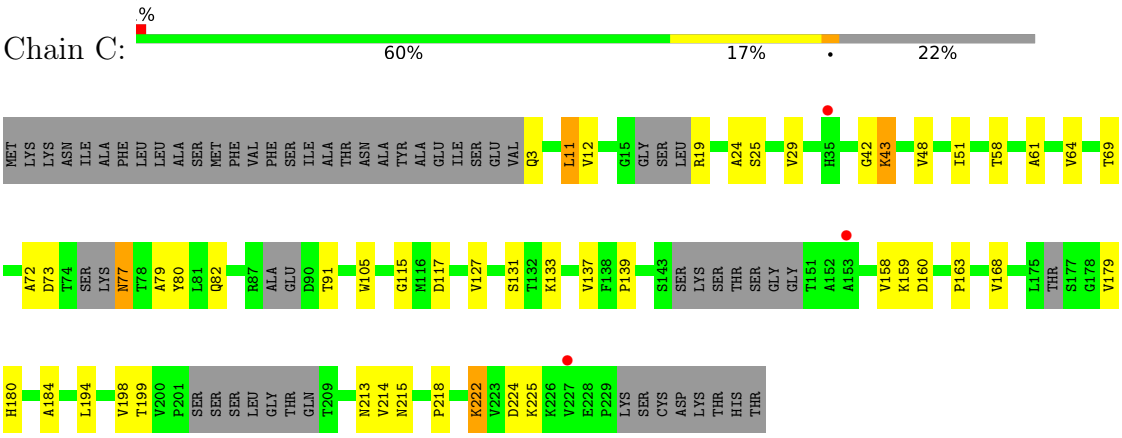
• Molecule 1: Insulin-degrading enzyme

Chain B:

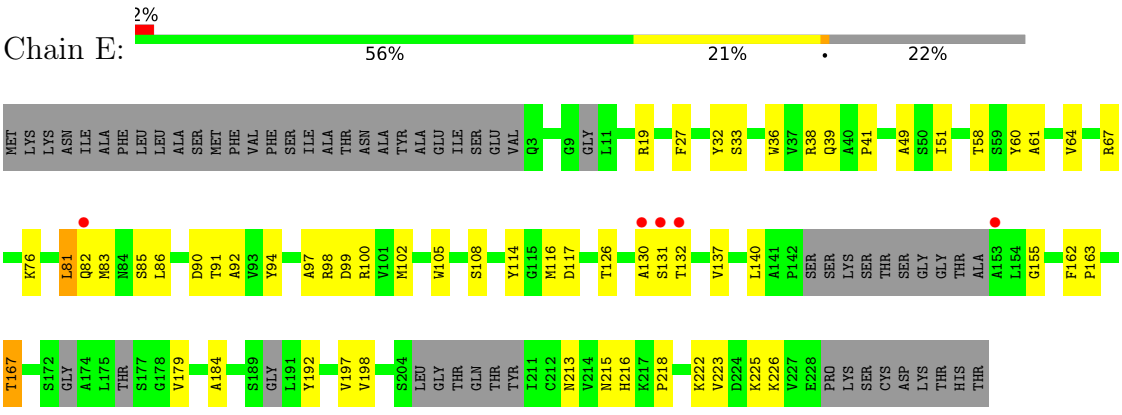




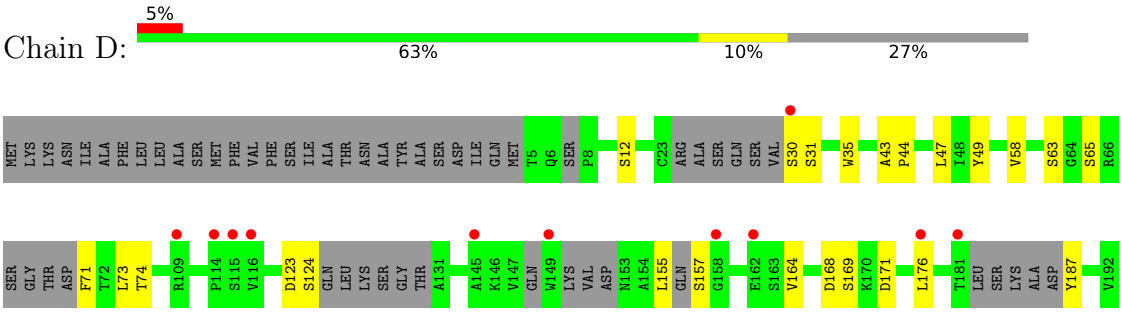
• Molecule 2: Fab-bound IDE, heavy chain

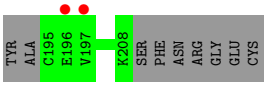


• Molecule 2: Fab-bound IDE, heavy chain



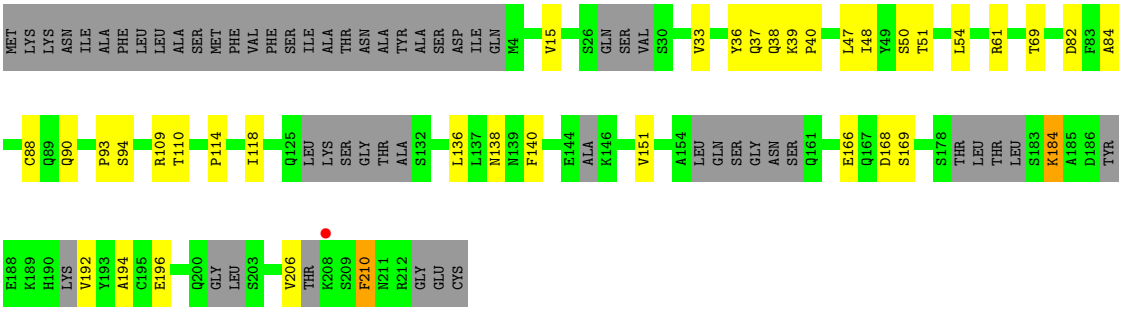
• Molecule 3: Fab-bound IDE, light chain





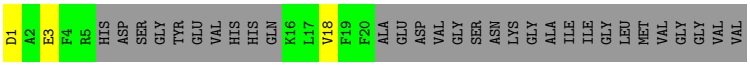
• Molecule 3: Fab-bound IDE, light chain

Chain F:



• Molecule 4: Amyloid beta A4 protein

Chain G:



• Molecule 4: Amyloid beta A4 protein

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.58Å 135.32Å 368.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 3.50 49.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.06-3.50) 92.6 (49.84-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.228 , 0.270 0.231 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (5.62%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 1.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	21509	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.22	0/7974	0.37	1/10793 (0.0%)
1	B	0.23	0/7938	0.38	1/10743 (0.0%)
2	C	0.20	0/1602	0.40	1/2179 (0.0%)
2	E	0.21	0/1605	0.39	0/2180
3	D	0.22	0/1362	0.44	0/1839
3	F	0.23	0/1433	0.41	0/1931
4	G	0.26	0/85	0.34	0/111
4	H	0.18	0/21	0.32	0/27
All	All	0.22	0/22020	0.39	3/29803 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	GLU	N-CA-C	5.98	127.16	111.00
2	C	43	LYS	N-CA-CB	5.80	121.04	110.60
1	B	564	ASP	CB-CA-C	-5.01	100.37	110.40

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	7779	0	7689	92	0
1	B	7745	0	7654	99	0
2	C	1562	0	1501	34	0
2	E	1567	0	1503	38	0
3	D	1339	0	1306	11	0
3	F	1409	0	1351	21	0
4	G	84	0	78	2	0
4	H	22	0	17	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	21509	0	21099	289	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 7.

All (289) 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:B:510:ILE:O	1:B:514:GLN:HG3	1.65	0.97
1:B:862:ARG:HH12	1:B:981:SER:HB2	1.38	0.87
1:B:510:ILE:HG22	1:B:514:GLN:HE21	1.47	0.79
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.71	0.73
1:A:339:GLY:O	4:G:1:ASP:N	2.21	0.73
1:A:429:ARG:HD3	1:A:898:LYS:HE2	1.71	0.73
1:B:341:GLU:HG3	1:B:347:LEU:HD23	1.71	0.73
1:B:510:ILE:HG22	1:B:514:GLN:NE2	2.06	0.70
2:C:139:PRO:HD3	2:C:225:LYS:HZ2	1.56	0.69
2:E:51:ILE:HG13	2:E:58:THR:HG22	1.74	0.68
2:E:38:ARG:NH1	2:E:90:ASP:OD1	2.29	0.66
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.78	0.66
2:C:213:ASN:ND2	2:C:224:ASP:OD1	2.25	0.65
1:B:862:ARG:NH1	1:B:981:SER:HB2	2.11	0.65
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.78	0.65
2:E:19:ARG:HG2	2:E:82:GLN:HA	1.80	0.64
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.78	0.64
1:B:839:ARG:HG2	1:B:844:GLN:HG2	1.79	0.64
3:F:61:ARG:NE	3:F:82:ASP:OD2	2.31	0.64
1:A:143:SER:HB3	1:A:146:HIS:HB2	1.80	0.63
1:B:946:VAL:HA	1:B:951:ARG:NH1	2.14	0.63
1:B:510:ILE:CG2	1:B:514:GLN:HE21	2.11	0.63
1:B:388:GLU:O	1:B:513:TRP:CH2	2.52	0.63
3:F:151:VAL:HA	3:F:194:ALA:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:179:VAL:HG12	2:C:180:HIS:H	1.65	0.62
1:B:777:PHE:HB2	1:B:954:VAL:HG23	1.83	0.61
1:A:782:ARG:NH1	1:A:963:MET:O	2.32	0.61
1:B:247:ALA:HA	1:B:281:LYS:NZ	2.16	0.60
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.83	0.60
2:E:39:GLN:OE1	3:F:38:GLN:NE2	2.33	0.60
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.83	0.60
2:C:24:ALA:O	2:C:77:ASN:ND2	2.35	0.60
2:C:222:LYS:NZ	2:C:222:LYS:HB3	2.17	0.60
2:E:91:THR:HG23	2:E:126:THR:HA	1.84	0.59
2:C:42:GLY:O	2:C:43:LYS:HD2	2.02	0.59
1:B:540:LEU:HD21	1:B:565:ASP:HB3	1.84	0.59
1:B:886:ILE:HG23	1:B:928:LEU:HG	1.85	0.59
2:E:137:VAL:HG11	2:E:223:VAL:HG21	1.85	0.59
1:A:877:MET:SD	1:A:933:LYS:NZ	2.76	0.59
1:B:564:ASP:CG	1:B:564:ASP:O	2.41	0.59
1:B:565:ASP:OD1	1:B:565:ASP:N	2.35	0.58
1:A:838:ARG:HB2	1:A:847:ARG:HD3	1.84	0.58
1:B:181:ARG:NH1	1:B:825:THR:O	2.36	0.58
2:E:155:GLY:HA3	2:E:197:VAL:HA	1.86	0.58
3:D:65:SER:O	3:D:71:PHE:N	2.37	0.58
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.86	0.57
1:B:175:ASP:OD1	1:B:176:GLU:N	2.37	0.57
1:A:574:LEU:HD22	1:A:729:LEU:HG	1.85	0.57
2:C:115:GLY:H	3:D:49:TYR:HB2	1.69	0.57
3:D:47:LEU:HA	3:D:58:VAL:HG21	1.86	0.57
2:E:49:ALA:HA	2:E:60:TYR:HA	1.87	0.56
1:A:591:ASN:ND2	1:A:700:LEU:O	2.38	0.56
1:A:441:LEU:HD12	1:A:449:VAL:HG11	1.88	0.56
1:A:777:PHE:HB3	1:A:992:ILE:HD11	1.86	0.56
1:B:130:PHE:O	1:B:134:HIS:ND1	2.32	0.56
1:B:579:PHE:HB2	1:B:724:HIS:HB3	1.86	0.56
1:B:591:ASN:ND2	1:B:700:LEU:O	2.37	0.56
1:B:774:ARG:HH21	1:B:949:PRO:HA	1.69	0.56
1:B:838:ARG:HB2	1:B:847:ARG:HD3	1.87	0.56
3:F:114:PRO:HG3	3:F:140:PHE:HB3	1.86	0.56
1:A:124:GLU:OE2	1:A:181:ARG:NH2	2.39	0.56
1:B:548:PRO:HB3	1:B:562:LYS:HB2	1.88	0.56
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.87	0.56
2:C:137:VAL:O	2:C:225:LYS:NZ	2.33	0.56
1:A:304:ILE:HB	1:A:481:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HG22	2:C:127:VAL:H	1.71	0.55
1:B:852:SER:OG	1:B:853:GLU:N	2.40	0.55
1:A:364:LYS:HB3	1:A:372:PHE:HB2	1.87	0.55
1:B:319:ILE:HD13	1:B:373:PHE:HB2	1.88	0.55
1:A:631:VAL:HG12	1:A:638:GLN:HE21	1.71	0.55
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.71	0.54
1:A:360:VAL:O	1:A:376:ASN:N	2.40	0.54
1:A:881:ALA:HA	1:A:884:LYS:HD3	1.89	0.54
2:C:131:SER:HB2	2:C:133:LYS:HE2	1.89	0.54
3:D:164:VAL:HG22	3:D:176:LEU:HD13	1.90	0.54
1:A:210:ASN:OD1	1:A:212:LYS:NZ	2.35	0.54
1:A:294:GLN:H	1:A:297:HIS:HB2	1.72	0.53
1:B:795:TYR:HE2	1:B:951:ARG:HH21	1.55	0.53
1:A:110:LEU:HD11	1:A:245:HIS:HB2	1.89	0.53
2:C:163:PRO:HD2	2:C:218:PRO:HB2	1.90	0.53
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.91	0.53
1:B:305:VAL:HB	1:B:499:GLN:HB2	1.91	0.53
2:C:61:ALA:HB3	2:C:64:VAL:HG22	1.91	0.53
2:E:213:ASN:HB3	2:E:222:LYS:NZ	2.24	0.53
1:A:319:ILE:HD13	1:A:373:PHE:HB2	1.89	0.52
1:A:690:MET:HB3	1:A:768:GLU:HG3	1.92	0.52
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.92	0.52
1:A:58:PRO:HG2	1:A:423:ARG:HH11	1.74	0.52
2:E:76:LYS:NZ	2:E:76:LYS:HB3	2.24	0.52
2:E:179:VAL:HA	2:E:198:VAL:HG22	1.90	0.52
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.91	0.52
1:A:941:LYS:HA	1:A:945:ALA:HB2	1.91	0.52
2:E:61:ALA:HB3	2:E:64:VAL:HG22	1.90	0.52
1:A:309:ASP:HA	1:A:483:LYS:HG3	1.92	0.52
1:A:361:GLY:O	4:G:3:GLU:HB2	2.10	0.52
1:A:557:SER:OG	1:A:746:GLU:OE1	2.24	0.52
2:C:179:VAL:HG23	2:C:198:VAL:HG23	1.92	0.52
2:C:29:VAL:HG23	2:C:77:ASN:HB2	1.92	0.52
2:C:159:LYS:HG2	2:C:160:ASP:OD1	2.10	0.52
3:F:196:GLU:HG3	3:F:206:VAL:HG22	1.92	0.51
3:F:118:ILE:HD13	3:F:210:PHE:HB3	1.92	0.51
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.92	0.51
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.92	0.51
3:F:50:SER:O	3:F:51:THR:HG22	2.11	0.51
1:B:294:GLN:HG2	1:B:295:GLU:H	1.76	0.51
1:B:388:GLU:O	1:B:513:TRP:HH2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:HH11	1:A:898:LYS:HE2	1.74	0.50
1:A:729:LEU:HB3	1:A:733:ILE:HD11	1.94	0.50
1:B:346:LEU:HD21	1:B:394:MET:HG2	1.92	0.50
2:E:33:SER:HB2	2:E:99:ASP:OD2	2.12	0.50
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.92	0.50
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.93	0.50
3:D:168:ASP:OD1	3:D:169:SER:N	2.44	0.50
2:E:184:ALA:HB1	2:E:192:TYR:HB3	1.93	0.50
1:A:946:VAL:HA	1:A:951:ARG:NH1	2.27	0.49
1:B:491:ARG:HH21	1:B:502:GLN:HB3	1.76	0.49
2:C:139:PRO:CD	2:C:225:LYS:HZ2	2.23	0.49
1:A:809:GLU:OE2	1:A:839:ARG:NH2	2.40	0.49
1:B:109:PHE:HD1	1:B:186:VAL:HG21	1.78	0.49
1:B:247:ALA:HA	1:B:281:LYS:HZ3	1.77	0.49
1:B:651:THR:HG23	1:B:752:HIS:HB3	1.95	0.49
2:E:197:VAL:HG11	3:F:136:LEU:HD22	1.94	0.49
1:B:791:ILE:HD11	1:B:860:GLU:OE2	2.12	0.49
1:A:48:LYS:HD3	1:A:70:ALA:HA	1.94	0.49
1:A:418:ASN:HB3	1:A:454:TYR:O	2.12	0.49
1:B:925:VAL:HG12	1:B:929:LYS:HE2	1.94	0.49
2:C:168:VAL:HG22	2:C:214:VAL:HG22	1.93	0.49
1:B:596:TYR:OH	1:B:649:MET:O	2.31	0.49
1:A:596:TYR:OH	1:A:649:MET:O	2.31	0.48
1:B:782:ARG:HH12	1:B:963:MET:H	1.61	0.48
1:B:823:LEU:HD13	1:B:850:ILE:HD11	1.93	0.48
1:A:604:LEU:HD21	1:A:648:LYS:HG2	1.95	0.48
1:B:928:LEU:HD12	1:B:931:LEU:HD12	1.94	0.48
1:A:413:GLU:OE2	1:A:528:ASN:HB2	2.13	0.48
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.95	0.48
1:B:768:GLU:HB3	1:B:843:ILE:HG13	1.96	0.48
1:A:810:LEU:HD23	1:A:936:ILE:HD11	1.95	0.48
2:C:179:VAL:HG21	2:C:199:THR:H	1.79	0.48
1:A:749:LEU:HB3	1:A:755:THR:HG21	1.96	0.48
2:E:97:ALA:HB1	2:E:116:MET:HB2	1.95	0.48
1:A:301:LEU:HG	1:A:505:ILE:HG23	1.95	0.48
1:A:916:TYR:HD2	1:A:1010:PRO:HB3	1.79	0.48
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.95	0.48
1:A:651:THR:HG23	1:A:752:HIS:HB3	1.96	0.48
1:A:139:ASN:OD1	1:A:140:ALA:N	2.44	0.47
3:F:15:VAL:HG12	3:F:109:ARG:HD2	1.96	0.47
1:B:335:GLY:HA2	1:B:362:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:SER:OG	3:D:74:THR:OG1	2.32	0.47
1:A:314:TYR:HB2	1:A:479:ALA:HB3	1.97	0.47
1:B:356:VAL:HA	1:B:379:LEU:HA	1.96	0.47
1:B:363:GLN:HA	1:B:373:PHE:HA	1.96	0.47
2:E:36:TRP:CD2	2:E:81:LEU:HD12	2.50	0.47
2:E:167:THR:HG23	2:E:215:ASN:HB3	1.96	0.47
1:B:213:HIS:CE1	1:B:292:PRO:HG3	2.50	0.47
1:A:643:LYS:HB2	1:A:643:LYS:NZ	2.30	0.46
2:C:42:GLY:O	2:C:43:LYS:CD	2.63	0.46
2:C:51:ILE:HG13	2:C:58:THR:HG22	1.96	0.46
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.96	0.46
1:A:465:GLU:HG2	2:C:105:TRP:HZ3	1.81	0.46
1:B:364:LYS:HB3	1:B:372:PHE:HB2	1.97	0.46
1:B:388:GLU:HG3	1:B:513:TRP:CH2	2.51	0.46
1:A:864:GLU:OE2	1:A:953:LYS:NZ	2.35	0.46
1:A:940:TYR:O	1:A:945:ALA:N	2.49	0.46
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.98	0.46
1:A:94:ILE:O	1:A:147:THR:OG1	2.26	0.46
2:E:27:PHE:CZ	2:E:98:ARG:HD2	2.51	0.46
2:E:130:ALA:HA	2:E:131:SER:HA	1.71	0.46
3:F:48:ILE:HG12	3:F:54:LEU:HD23	1.98	0.46
1:B:364:LYS:HD3	1:B:374:ILE:HD13	1.97	0.46
1:A:782:ARG:NH2	1:A:965:SER:OG	2.49	0.45
1:A:298:LEU:HD21	1:A:318:PRO:HG3	1.97	0.45
1:B:387:VAL:HG21	1:B:480:ILE:HD12	1.98	0.45
2:C:11:LEU:HD23	2:C:11:LEU:H	1.81	0.45
3:F:33:VAL:HG23	3:F:90:GLN:HB3	1.98	0.45
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.98	0.45
2:C:3:GLN:N	2:C:25:SER:O	2.49	0.45
1:A:852:SER:OG	1:A:853:GLU:N	2.49	0.45
2:E:100:ARG:NH1	2:E:114:TYR:HB3	2.31	0.45
1:A:49:ARG:HG2	1:A:68:GLU:HB3	1.98	0.45
2:E:225:LYS:HB3	2:E:226:LYS:HB2	1.99	0.45
1:B:119:LYS:HD3	1:B:171:SER:O	2.17	0.45
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.51	0.45
2:C:117:ASP:N	2:C:117:ASP:OD1	2.44	0.45
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.98	0.44
1:B:94:ILE:O	1:B:147:THR:OG1	2.26	0.44
1:B:722:ARG:HB3	1:B:758:LEU:HD12	1.99	0.44
2:C:139:PRO:HD3	2:C:225:LYS:NZ	2.28	0.44
1:B:62:ARG:HD3	1:B:427:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD23	1:B:437:ILE:HG21	1.99	0.44
1:A:180:ASP:O	1:A:184:ASN:ND2	2.50	0.44
1:B:465:GLU:HG2	2:E:105:TRP:HZ3	1.82	0.44
1:A:305:VAL:HG11	1:A:486:GLU:OE2	2.17	0.44
1:B:759:LEU:HD12	1:B:760:PRO:HD2	1.99	0.44
1:B:959:LEU:HD21	1:B:963:MET:HB2	2.00	0.44
3:D:43:ALA:HA	3:D:44:PRO:HD3	1.85	0.44
3:F:39:LYS:HD3	3:F:84:ALA:HB2	1.99	0.44
1:A:468:LEU:HD12	1:A:471:LEU:HD12	1.99	0.44
1:B:770:GLN:HB3	1:B:1003:PRO:HB2	1.99	0.44
2:E:116:MET:HG2	3:F:36:TYR:OH	2.18	0.44
1:A:579:PHE:HB2	1:A:724:HIS:HB3	1.99	0.44
2:C:137:VAL:HB	2:C:225:LYS:HE2	2.00	0.44
3:D:155:LEU:HG	3:D:157:SER:HB3	1.99	0.44
1:A:108:HIS:NE2	1:A:189:GLU:OE2	2.48	0.44
1:B:679:HIS:ND1	1:B:851:GLN:OE1	2.42	0.44
2:C:184:ALA:HA	2:C:194:LEU:HB3	2.00	0.44
2:C:72:ALA:HA	2:C:79:ALA:HA	2.00	0.44
1:A:224:TYR:HA	1:A:228:THR:HB	1.99	0.43
1:A:806:MET:HE3	1:A:928:LEU:HD13	2.01	0.43
2:E:32:TYR:CZ	2:E:102:MET:HG2	2.54	0.43
2:E:162:PHE:HA	2:E:163:PRO:HA	1.83	0.43
1:B:945:ALA:HB3	1:B:948:ALA:HB2	1.99	0.43
2:E:140:LEU:HB3	2:E:155:GLY:O	2.18	0.43
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.87	0.43
1:B:214:PRO:HA	1:B:217:LYS:HE3	2.00	0.43
1:A:92:VAL:HG22	1:A:254:MET:HG2	2.00	0.43
1:B:792:GLU:HA	1:B:848:PHE:O	2.18	0.43
1:A:602:ASP:OD1	1:A:658:ARG:NH2	2.41	0.43
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.53	0.43
1:B:722:ARG:NH1	1:B:722:ARG:HB2	2.34	0.43
2:C:158:VAL:HB	2:C:194:LEU:HD23	2.00	0.43
3:F:168:ASP:OD1	3:F:169:SER:N	2.50	0.43
1:A:720:LEU:O	1:A:755:THR:HG22	2.18	0.43
1:A:898:LYS:H	1:A:898:LYS:HD2	1.83	0.43
1:B:417:LEU:HD21	1:B:531:ILE:HG12	2.01	0.43
2:C:69:THR:O	2:C:82:GLN:N	2.44	0.43
1:A:809:GLU:OE1	1:A:893:ARG:NH1	2.52	0.43
1:B:558:LYS:H	1:B:724:HIS:HE1	1.67	0.43
1:B:806:MET:SD	1:B:924:GLU:HB3	2.59	0.43
1:B:324:LYS:HD2	1:B:324:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:GLU:OE1	1:B:893:ARG:NH1	2.51	0.42
1:A:112:HIS:HB3	1:A:182:GLU:OE2	2.19	0.42
1:B:247:ALA:HA	1:B:281:LYS:HZ2	1.84	0.42
1:B:511:LYS:O	1:B:515:ASN:HB2	2.18	0.42
1:B:468:LEU:HD12	1:B:471:LEU:HD12	2.01	0.42
2:E:38:ARG:HD3	2:E:94:TYR:CE1	2.55	0.42
2:E:131:SER:OG	2:E:132:THR:N	2.51	0.42
3:F:40:PRO:HB2	3:F:166:GLU:HG3	2.02	0.42
1:A:104:ALA:HB1	1:A:218:PHE:HB3	2.01	0.42
1:B:210:ASN:HB3	1:B:213:HIS:HB2	2.01	0.42
1:A:882:PHE:HB2	1:A:933:LYS:HD2	2.01	0.42
1:A:916:TYR:CD2	1:A:1010:PRO:HB3	2.55	0.42
1:A:119:LYS:HE3	1:A:119:LYS:HB3	1.92	0.42
1:B:729:LEU:HD12	1:B:738:ALA:HB1	2.01	0.42
2:E:117:ASP:OD1	2:E:117:ASP:N	2.51	0.42
3:F:93:PRO:HA	3:F:94:SER:HA	1.70	0.42
1:A:789:SER:N	1:A:852:SER:O	2.42	0.42
1:B:884:LYS:HE3	1:B:884:LYS:HB2	1.83	0.41
2:C:73:ASP:OD1	2:C:80:TYR:HE2	2.03	0.41
2:E:67:ARG:HD2	2:E:85:SER:HB2	2.02	0.41
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.50	0.41
1:A:62:ARG:HD3	1:A:427:LYS:HE3	2.02	0.41
1:A:580:SER:HA	1:A:581:PRO:HD3	1.83	0.41
1:A:797:THR:HG22	1:A:798:ASP:H	1.84	0.41
1:B:341:GLU:HB3	1:B:609:TYR:CG	2.55	0.41
1:B:896:LYS:HA	1:B:897:PRO:HD3	1.93	0.41
2:E:27:PHE:CE1	2:E:98:ARG:HD2	2.56	0.41
1:B:524:LEU:HA	1:B:525:PRO:HD3	1.93	0.41
2:C:179:VAL:HB	2:C:198:VAL:HA	2.02	0.41
1:A:524:LEU:HA	1:A:525:PRO:HD3	1.95	0.41
2:C:222:LYS:HB3	2:C:222:LYS:HZ2	1.82	0.41
2:E:225:LYS:HA	2:E:226:LYS:HA	1.86	0.41
1:A:143:SER:OG	1:A:144:GLY:N	2.53	0.41
1:A:773:ASP:OD2	1:A:950:ARG:HG2	2.19	0.41
2:E:216:HIS:CD2	2:E:218:PRO:HD2	2.55	0.41
1:B:143:SER:HB3	1:B:146:HIS:HB2	2.01	0.41
1:B:776:TRP:CD1	1:B:989:PRO:HA	2.56	0.41
1:B:810:LEU:HD23	1:B:936:ILE:HD11	2.03	0.41
1:B:864:GLU:CD	1:B:951:ARG:HH22	2.23	0.41
1:A:49:ARG:HH21	1:A:446:LEU:HD13	1.86	0.41
2:E:130:ALA:HB1	2:E:131:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:151:VAL:HA	3:F:194:ALA:N	2.34	0.41
1:A:505:ILE:HA	1:A:506:PRO:HD3	1.95	0.41
1:B:124:GLU:OE2	1:B:181:ARG:NH2	2.52	0.41
1:B:580:SER:HA	1:B:581:PRO:HD3	1.85	0.41
3:D:123:ASP:OD1	3:D:124:SER:N	2.52	0.41
3:F:109:ARG:HB3	3:F:110:THR:H	1.76	0.41
3:F:184:LYS:H	3:F:184:LYS:HG3	1.67	0.41
1:A:210:ASN:HA	1:A:211:PRO:HD3	1.96	0.41
1:A:986:LEU:HA	1:A:987:PRO:HD3	1.89	0.41
1:B:58:PRO:HG2	1:B:423:ARG:HG3	2.03	0.41
3:F:138:ASN:OD1	3:F:138:ASN:N	2.52	0.41
1:B:789:SER:HB3	1:B:960:ALA:HB2	2.02	0.40
1:B:120:LYS:HE3	1:B:121:TYR:CE2	2.56	0.40
3:D:30:SER:OG	3:D:31:SER:N	2.55	0.40
2:E:38:ARG:HD3	2:E:94:TYR:CZ	2.55	0.40
1:A:599:LEU:HD13	1:A:654:ILE:HD12	2.03	0.40
1:B:238:ARG:NH1	1:B:242:LEU:HD11	2.36	0.40
2:C:137:VAL:C	2:C:225:LYS:NZ	2.74	0.40
3:D:35:TRP:CD2	3:D:73:LEU:HB2	2.57	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	951/990 (96%)	926 (97%)	23 (2%)	2 (0%)	47 81
1	B	946/990 (96%)	917 (97%)	29 (3%)	0	100 100
2	C	191/263 (73%)	183 (96%)	8 (4%)	0	100 100
2	E	192/263 (73%)	182 (95%)	10 (5%)	0	100 100
3	D	156/239 (65%)	147 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	164/239 (69%)	156 (95%)	8 (5%)	0	100 100
4	G	6/40 (15%)	5 (83%)	1 (17%)	0	100 100
4	H	1/40 (2%)	1 (100%)	0	0	100 100
All	All	2607/3064 (85%)	2517 (96%)	88 (3%)	2 (0%)	51 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	PRO
1	A	172	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	840/879 (96%)	835 (99%)	5 (1%)	86 94
1	B	837/879 (95%)	826 (99%)	11 (1%)	69 86
2	C	172/220 (78%)	165 (96%)	7 (4%)	30 63
2	E	173/220 (79%)	170 (98%)	3 (2%)	60 82
3	D	157/210 (75%)	154 (98%)	3 (2%)	57 80
3	F	162/210 (77%)	157 (97%)	5 (3%)	40 70
4	G	8/31 (26%)	7 (88%)	1 (12%)	4 23
4	H	2/31 (6%)	2 (100%)	0	100 100
All	All	2351/2680 (88%)	2316 (98%)	35 (2%)	65 84

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	PHE
1	A	423	ARG
1	A	449	VAL
1	A	797	THR

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Mol	Chain	Res	Type
1	A	898	LYS
1	B	291	HIS
1	B	379	LEU
1	B	441	LEU
1	B	458	GLU
1	B	513	TRP
1	B	515	ASN
1	B	564	ASP
1	B	565	ASP
1	B	567	PHE
1	B	722	ARG
1	B	959	LEU
2	C	11	LEU
2	C	12	VAL
2	C	19	ARG
2	C	48	VAL
2	C	77	ASN
2	C	215	ASN
2	C	222	LYS
3	D	12	SER
3	D	171	ASP
3	D	187	TYR
2	E	81	LEU
2	E	108	SER
2	E	167	THR
3	F	69	THR
3	F	88	CYS
3	F	184	LYS
3	F	192	VAL
3	F	210	PHE
4	G	18	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	514	GLN
1	B	515	ASN
1	B	677	GLN
2	C	77	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	957/990 (96%)	-0.31	1 (0%) 95 95	50, 73, 96, 117	0
1	B	952/990 (96%)	-0.37	0 100 100	48, 68, 88, 107	0
2	C	205/263 (77%)	0.27	3 (1%) 73 68	74, 104, 124, 136	0
2	E	206/263 (78%)	0.11	5 (2%) 59 53	69, 92, 114, 126	0
3	D	175/239 (73%)	0.36	13 (7%) 14 14	77, 102, 132, 143	0
3	F	184/239 (76%)	0.08	1 (0%) 91 88	71, 94, 117, 128	0
4	G	10/40 (25%)	0.04	0 100 100	81, 97, 109, 110	0
4	H	3/40 (7%)	-0.07	0 100 100	74, 74, 96, 98	0
All	All	2692/3064 (87%)	-0.18	23 (0%) 84 79	48, 76, 113, 143	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	153	ALA	3.6
2	E	131	SER	3.4
2	E	82	GLN	3.3
3	D	30	SER	2.8
2	E	132	THR	2.7
2	C	35	HIS	2.7
3	D	116	VAL	2.6
3	D	181	THR	2.5
2	E	130	ALA	2.5
3	D	114	PRO	2.5
3	D	109	ARG	2.4
3	D	176	LEU	2.4
3	F	208	LYS	2.4
3	D	149	TRP	2.3
2	C	227	VAL	2.3
3	D	115	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	145	ALA	2.3
3	D	197	VAL	2.2
1	A	379	LEU	2.2
3	D	158	GLY	2.2
3	D	196	GLU	2.1
2	E	153	ALA	2.1
3	D	162	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	B	2001	1/1	0.88	0.09	59,59,59,59	0
5	ZN	A	1101	1/1	0.98	0.12	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.