



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:44 PM UTC

PDB ID : 4J6L / pdb_00004j6l
Title : Crystal structure of calcium²⁺-free wild-type CD23 lectin domain (crystal form C)
Authors : Dhaliwal, B.; Yuan, D.; Sutton, B.J.
Deposited on : 2013-02-11
Resolution : 3.15 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:

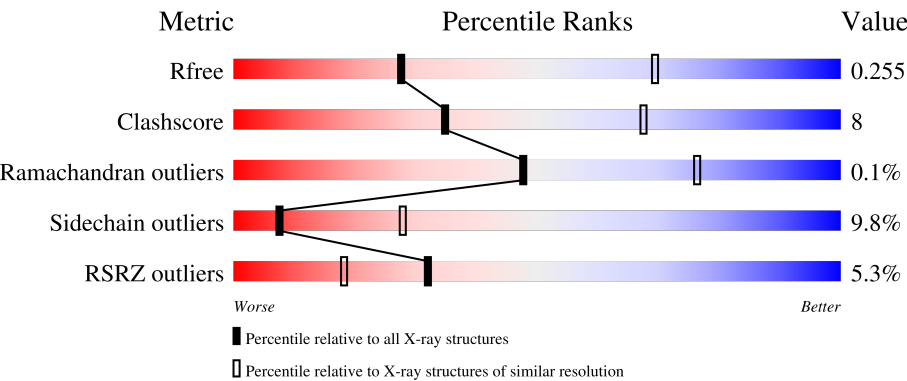
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	143	3% 71% 18% • • 7%
1	B	143	% 70% 20% • 7%
1	C	143	6% 71% 20% • 8%
1	D	143	8% 73% 18% • • 7%
1	E	143	7% 73% 17% • 9%

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Mol	Chain	Length	Quality of chain
1	F	143	5% 57% 29% • 10%
1	G	143	4% 70% 21% • 6%
1	H	143	5% 68% 20% •• 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8461 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 Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1069	671	190	197	11			
1	B	133	Total	C	N	O	S	0	0	0
			1065	667	190	197	11			
1	C	132	Total	C	N	O	S	0	0	0
			1061	665	189	196	11			
1	D	133	Total	C	N	O	S	0	0	0
			1071	672	191	197	11			
1	E	130	Total	C	N	O	S	0	0	0
			1042	652	187	192	11			
1	F	128	Total	C	N	O	S	0	0	0
			1028	643	183	191	11			
1	G	135	Total	C	N	O	S	0	0	0
			1082	679	193	199	11			
1	H	129	Total	C	N	O	S	0	0	0
			1039	649	187	192	11			

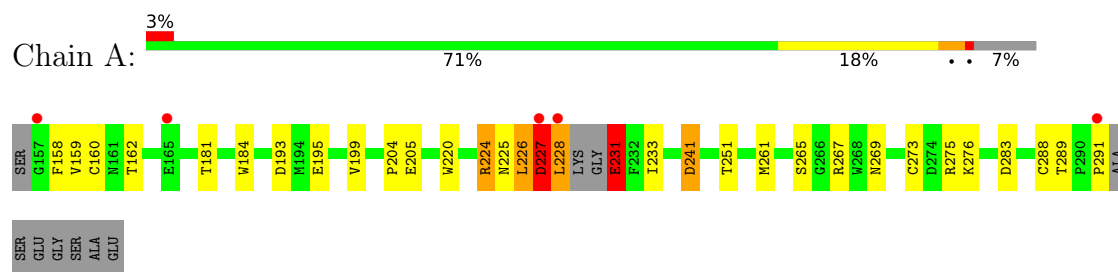
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	E	1	Total	O	0	0
			1	1		

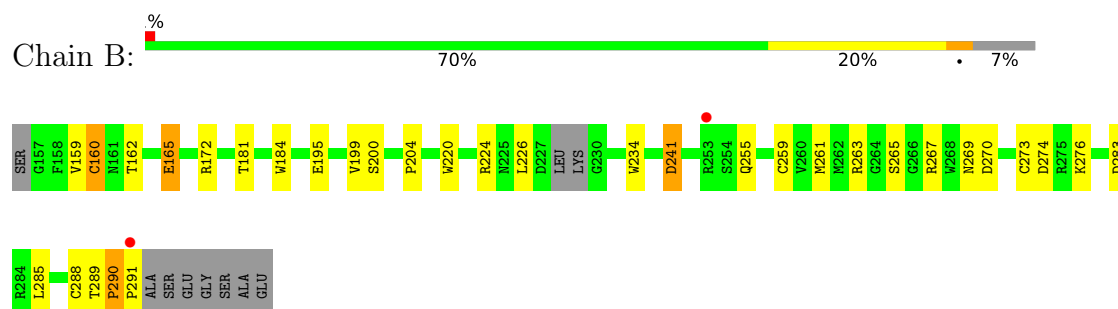
3 Residue-property plots [i](#)

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.

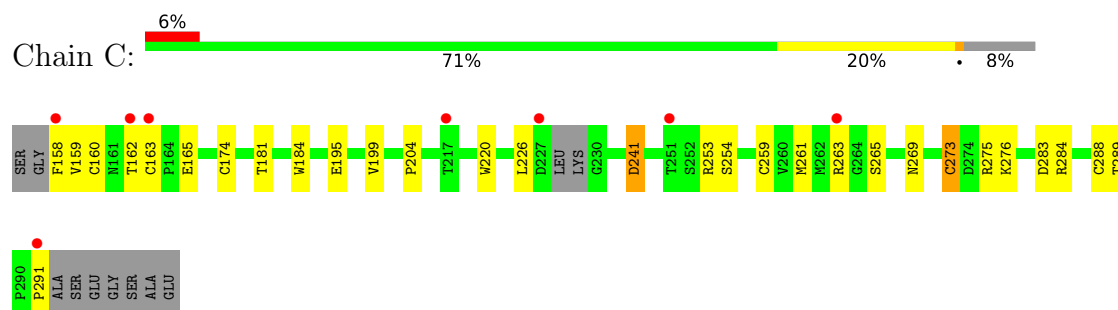
- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor



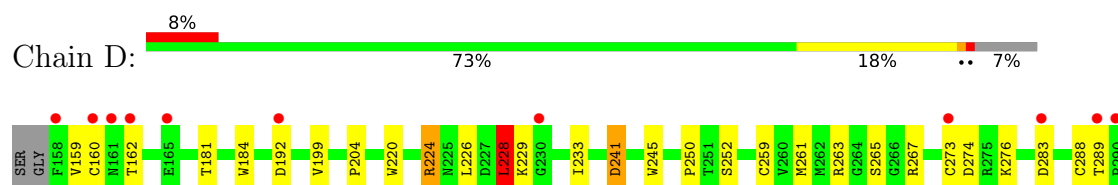
- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor



PRO
ALA
SER
GLY
SER
ALA
GLU

- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain E: 

SER GLY PHE V159 N160 N161 T162 C163 C174 T181 W184 D192 E195 V199 P204 H216 T217 W220 N224 N225 L226 ASP LEU LYS G230 E231 D241 T251 S252 R253 S254 Q255 M261 S265 N269 D270 C273 D274 R275 K276 D283 R284

C288 T289 P290 P291 ALA SER GLY SER ALA GLU

- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain F: 

SER GLY PHE VAL C160 N161 T162 C163 P164 E165 N169 C174 T181 K182 Q183 W184 D192 D193 M194 E195 G196 Q197 L198 V199 S200 I201 P204 E205 D208 F209 L210 W220 L223 R224 N225 L226 D227 L228 K229 G230 E231 F232 I233 W234 D241 W245 P250 S252

ARG S264 Q265 V260 M261 G264 C273 K276 C282 D283 C288 THR PRO ALA SER GLY SER ALA GLU

- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain G: 

SER G157 F158 V159 C160 N161 E165 T181 W184 D192 E195 V199 S200 I201 P204 L210 W220 N225 L226 G230 E231 W234 D241 W245 P250 V260 M261 N262 R263 G264 S265 N269 D270 C273 K276 L277 D283 C288 T289

P290 P291 ALA SER GLY SER ALA GLU

- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain H: 

SER GLY PHE VAL C160 C163 T181 K182 W184 D192 D193 M194 E195 V199 S200 I201 P204 D208 F209 L210 W220 N225 L226 D227 L228 F232 T233 W234 D241 T251 S252 R253 S254 Q255 E257 M261 R262 R263 G264 S265 N269 C273 K276

D283 C288 THR PRO ALA SER GLY SER ALA GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.26Å 64.33Å 112.20Å 75.28° 82.39° 89.95°	Depositor
Resolution (Å)	49.36 – 3.15 49.36 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.36-3.15) 96.7 (49.36-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.212 , 0.253 0.228 , 0.255	Depositor DCC
R_{free} test set	1193 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8461	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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	0.81	0/1102	1.43	16/1493 (1.1%)
1	B	0.83	1/1098 (0.1%)	1.34	11/1487 (0.7%)
1	C	0.79	0/1094	1.27	7/1482 (0.5%)
1	D	0.83	1/1104 (0.1%)	1.33	10/1495 (0.7%)
1	E	0.84	0/1074	1.34	9/1455 (0.6%)
1	F	0.91	1/1058 (0.1%)	1.44	18/1430 (1.3%)
1	G	0.82	0/1116	1.47	11/1512 (0.7%)
1	H	0.80	0/1070	1.39	14/1447 (1.0%)
All	All	0.83	3/8716 (0.0%)	1.38	96/11801 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	THR	C-N	7.79	1.44	1.33
1	B	226	LEU	CA-C	6.29	1.58	1.52
1	D	228	LEU	CA-C	-5.24	1.46	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	231	GLU	N-CA-C	20.74	136.94	111.02
1	A	227	ASP	CB-CA-C	14.88	133.94	109.99
1	H	255	GLN	CB-CA-C	13.57	137.43	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	N-CA-C	-12.69	89.23	108.52
1	F	251	THR	N-CA-C	-10.24	99.94	111.82
1	D	228	LEU	N-CA-C	-9.26	97.44	110.50
1	A	227	ASP	CA-C-N	-8.44	106.51	121.70
1	A	227	ASP	C-N-CA	-8.44	106.51	121.70
1	F	254	SER	CA-C-N	7.87	135.86	121.70
1	F	254	SER	C-N-CA	7.87	135.86	121.70
1	F	231	GLU	N-CA-C	7.24	126.22	110.80
1	B	270	ASP	CA-CB-CG	7.00	119.60	112.60
1	G	270	ASP	CA-CB-CG	6.81	119.41	112.60
1	F	283	ASP	CA-CB-CG	6.80	119.40	112.60
1	H	283	ASP	CA-CB-CG	6.79	119.39	112.60
1	G	283	ASP	CA-CB-CG	6.74	119.33	112.60
1	A	283	ASP	CA-CB-CG	6.70	119.30	112.60
1	G	231	GLU	CB-CA-C	-6.66	100.05	112.30
1	D	283	ASP	CA-CB-CG	6.57	119.17	112.60
1	D	288	CYS	N-CA-C	6.41	119.56	110.14
1	E	252	SER	CA-C-N	6.34	129.41	120.28
1	E	252	SER	C-N-CA	6.34	129.41	120.28
1	B	241	ASP	N-CA-C	-6.28	101.48	111.02
1	F	264	GLY	CA-C-N	6.23	129.47	120.38
1	F	264	GLY	C-N-CA	6.23	129.47	120.38
1	E	283	ASP	CA-CB-CG	6.22	118.83	112.60
1	B	283	ASP	CA-CB-CG	6.19	118.79	112.60
1	G	192	ASP	CA-CB-CG	6.17	118.77	112.60
1	C	283	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	241	ASP	CA-CB-CG	6.10	118.70	112.60
1	E	288	CYS	N-CA-C	6.07	119.06	110.14
1	A	251	THR	CB-CA-C	6.02	119.29	110.26
1	B	269	ASN	CA-CB-CG	6.01	118.61	112.60
1	D	204	PRO	CA-C-N	5.96	128.26	120.28
1	D	204	PRO	C-N-CA	5.96	128.26	120.28
1	F	204	PRO	CA-C-N	5.96	128.26	120.28
1	F	204	PRO	C-N-CA	5.96	128.26	120.28
1	G	204	PRO	CA-C-N	5.92	128.21	120.28
1	G	204	PRO	C-N-CA	5.92	128.21	120.28
1	B	204	PRO	CA-C-N	5.90	128.19	120.28
1	B	204	PRO	C-N-CA	5.90	128.19	120.28
1	F	199	VAL	N-CA-C	5.88	117.00	109.30
1	E	192	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	199	VAL	N-CA-C	5.83	116.94	109.30
1	G	199	VAL	N-CA-C	5.83	116.93	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	SER	CA-C-N	5.80	129.00	120.82
1	D	252	SER	C-N-CA	5.80	129.00	120.82
1	H	199	VAL	N-CA-C	5.75	116.83	109.30
1	E	204	PRO	CA-C-N	5.66	127.87	120.28
1	E	204	PRO	C-N-CA	5.66	127.87	120.28
1	F	192	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	259	CYS	N-CA-C	5.58	119.02	110.20
1	D	199	VAL	N-CA-C	5.58	116.60	109.30
1	H	227	ASP	CA-C-N	5.57	128.51	120.38
1	H	227	ASP	C-N-CA	5.57	128.51	120.38
1	B	288	CYS	N-CA-C	5.55	118.29	110.14
1	F	162	THR	N-CA-C	5.55	117.74	109.25
1	G	288	CYS	N-CA-C	5.54	118.73	110.14
1	E	231	GLU	CB-CG-CD	5.50	121.95	112.60
1	C	204	PRO	CA-C-N	5.49	127.64	120.28
1	C	204	PRO	C-N-CA	5.49	127.64	120.28
1	A	204	PRO	CA-C-N	5.47	127.62	120.28
1	A	204	PRO	C-N-CA	5.47	127.62	120.28
1	C	269	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	199	VAL	N-CA-C	5.46	116.45	109.30
1	H	254	SER	CA-C-N	5.40	131.85	121.54
1	H	254	SER	C-N-CA	5.40	131.85	121.54
1	A	288	CYS	N-CA-C	5.39	118.49	110.14
1	E	199	VAL	N-CA-C	5.39	116.36	109.30
1	C	199	VAL	N-CA-C	5.38	116.35	109.30
1	A	241	ASP	N-CA-C	-5.36	104.78	112.13
1	A	269	ASN	CA-CB-CG	5.36	117.96	112.60
1	H	192	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	241	ASP	N-CA-C	-5.30	104.87	112.13
1	H	241	ASP	N-CA-C	-5.30	104.87	112.13
1	B	290	PRO	N-CA-C	5.28	117.14	110.70
1	F	241	ASP	N-CA-C	-5.27	104.91	112.13
1	F	162	THR	CB-CA-C	5.23	118.86	110.29
1	H	255	GLN	CA-C-N	5.21	131.63	121.41
1	H	255	GLN	C-N-CA	5.21	131.63	121.41
1	D	192	ASP	CA-CB-CG	5.18	117.78	112.60
1	G	269	ASN	CA-C-N	-5.17	115.52	122.86
1	G	269	ASN	C-N-CA	-5.17	115.52	122.86
1	C	288	CYS	N-CA-C	5.15	118.12	110.14
1	F	228	LEU	CA-C-N	5.14	131.36	121.54
1	F	228	LEU	C-N-CA	5.14	131.36	121.54
1	A	205	GLU	CA-C-N	5.12	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLU	C-N-CA	5.12	127.09	120.44
1	H	255	GLN	N-CA-C	-5.11	99.92	110.80
1	H	204	PRO	CA-C-N	5.10	127.12	120.28
1	H	204	PRO	C-N-CA	5.10	127.12	120.28
1	A	231	GLU	CA-C-N	5.10	129.19	122.30
1	A	231	GLU	C-N-CA	5.10	129.19	122.30
1	F	205	GLU	CA-C-N	5.06	127.32	120.44
1	F	205	GLU	C-N-CA	5.06	127.32	120.44
1	D	241	ASP	N-CA-C	-5.06	105.20	112.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ASP	Peptide
1	H	255	GLN	Peptide

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	1069	0	983	33	3
1	B	1065	0	975	10	0
1	C	1061	0	972	10	0
1	D	1071	0	992	17	0
1	E	1042	0	959	4	0
1	F	1028	0	946	22	0
1	G	1082	0	1000	12	1
1	H	1039	0	958	22	4
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	8461	0	7785	120	4

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 (120) 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:A:226:LEU:HD22	1:A:226:LEU:N	1.58	1.14
1:D:229:LYS:HE3	1:F:254:SER:N	1.78	0.96
1:A:227:ASP:CA	1:A:228:LEU:C	2.35	0.94
1:D:228:LEU:O	1:D:229:LYS:HB2	1.67	0.93
1:A:226:LEU:N	1:A:226:LEU:CD2	2.32	0.93
1:A:227:ASP:C	1:A:228:LEU:HD13	1.95	0.92
1:F:163:CYS:HG	1:F:174:CYS:HG	1.18	0.92
1:A:226:LEU:HD22	1:A:226:LEU:H	1.21	0.91
1:A:227:ASP:O	1:A:228:LEU:HD13	1.71	0.90
1:H:253:ARG:O	1:H:255:GLN:N	2.05	0.90
1:A:228:LEU:CD1	1:A:228:LEU:N	2.34	0.89
1:A:228:LEU:CD2	1:A:231:GLU:HG2	2.07	0.84
1:A:224:ARG:HG3	1:A:225:ASN:N	1.97	0.80
1:H:252:SER:O	1:H:253:ARG:CG	2.30	0.79
1:A:228:LEU:N	1:A:228:LEU:HD12	1.97	0.79
1:D:228:LEU:O	1:D:229:LYS:CB	2.30	0.78
1:A:226:LEU:CD2	1:A:226:LEU:H	1.94	0.78
1:A:228:LEU:CD2	1:A:231:GLU:HB3	2.14	0.77
1:A:228:LEU:HD22	1:A:231:GLU:HB3	1.67	0.77
1:A:227:ASP:HA	1:A:228:LEU:C	2.10	0.74
1:D:228:LEU:H	1:D:228:LEU:HD23	1.54	0.73
1:F:160:CYS:HB3	1:F:288:CYS:SG	2.31	0.71
1:A:227:ASP:C	1:A:228:LEU:CD1	2.64	0.69
1:H:252:SER:O	1:H:253:ARG:HG3	1.92	0.68
1:F:231:GLU:O	1:F:231:GLU:HG3	1.94	0.66
1:F:226:LEU:HD13	1:F:233:ILE:HG13	1.77	0.66
1:B:165:GLU:OE2	2:B:301:HOH:O	2.13	0.66
1:A:225:ASN:OD1	1:A:226:LEU:N	2.29	0.65
1:A:227:ASP:O	1:A:228:LEU:CD1	2.45	0.65
1:H:253:ARG:C	1:H:254:SER:OG	2.30	0.65
1:G:261:MET:HE2	1:G:277:LEU:HD21	1.82	0.62
1:H:253:ARG:C	1:H:254:SER:HG	2.05	0.61
1:F:231:GLU:O	1:F:231:GLU:CG	2.47	0.61
1:A:228:LEU:CD2	1:A:231:GLU:CB	2.79	0.60
1:A:228:LEU:CD2	1:A:231:GLU:CG	2.78	0.60
1:H:263:ARG:HG3	1:H:269:ASN:ND2	2.17	0.60
1:D:184:TRP:CG	1:D:259:CYS:HG	2.21	0.59
1:B:274:ASP:OD2	1:D:224:ARG:NH2	2.36	0.58
1:A:228:LEU:HD23	1:A:231:GLU:CB	2.33	0.58
1:A:275:ARG:HG3	1:G:226:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ARG:HG3	1:H:226:LEU:HD23	1.87	0.57
1:A:228:LEU:HD23	1:A:231:GLU:CG	2.35	0.57
1:A:227:ASP:N	1:A:228:LEU:C	2.63	0.56
1:H:252:SER:O	1:H:253:ARG:HG2	2.03	0.56
1:H:252:SER:C	1:H:253:ARG:HG3	2.31	0.55
1:E:275:ARG:HD2	1:F:226:LEU:HD23	1.89	0.54
1:A:226:LEU:HD11	1:A:233:ILE:HG13	1.88	0.54
1:F:183:GLN:HE21	1:F:276:LYS:NZ	2.07	0.52
1:G:263:ARG:HG3	1:G:269:ASN:ND2	2.24	0.51
1:A:225:ASN:C	1:A:226:LEU:HD22	2.32	0.51
1:A:228:LEU:HD22	1:A:231:GLU:HG2	1.93	0.50
1:F:225:ASN:OD1	1:F:230:GLY:O	2.31	0.49
1:A:181:THR:HG23	1:A:276:LYS:HB3	1.94	0.49
1:A:224:ARG:HG3	1:A:225:ASN:H	1.76	0.49
1:D:226:LEU:HD23	1:D:233:ILE:HG13	1.93	0.48
1:H:181:THR:HG23	1:H:276:LYS:HB3	1.96	0.48
1:F:163:CYS:SG	1:F:169:ASN:HB2	2.53	0.48
1:H:225:ASN:HB2	1:H:232:PHE:CE2	2.49	0.48
1:A:184:TRP:HD1	1:A:220:TRP:CE3	2.31	0.47
1:F:181:THR:HG23	1:F:276:LYS:HB3	1.96	0.47
1:B:181:THR:HG23	1:B:276:LYS:HB3	1.96	0.47
1:B:160:CYS:HB2	1:B:172:ARG:HG3	1.97	0.47
1:D:181:THR:HG23	1:D:276:LYS:HB3	1.97	0.46
1:D:245:TRP:CG	1:D:250:PRO:HD3	2.50	0.46
1:C:254:SER:HB3	1:H:256:GLY:HA2	1.97	0.46
1:F:245:TRP:CE2	1:F:250:PRO:HG3	2.51	0.46
1:B:255:GLN:HG3	1:D:274:ASP:HB3	1.98	0.46
1:E:181:THR:HG23	1:E:276:LYS:HB3	1.97	0.45
1:E:184:TRP:HD1	1:E:220:TRP:CE3	2.33	0.45
1:G:181:THR:HG23	1:G:276:LYS:HB3	1.98	0.45
1:F:184:TRP:HD1	1:F:220:TRP:CE3	2.35	0.45
1:C:181:THR:HG23	1:C:276:LYS:HB3	1.98	0.45
1:D:263:ARG:HH11	1:D:267:ARG:NH2	2.15	0.45
1:F:227:ASP:C	1:F:229:LYS:H	2.25	0.45
1:G:184:TRP:HD1	1:G:220:TRP:CE3	2.33	0.45
1:H:251:THR:O	1:H:251:THR:OG1	2.30	0.45
1:H:253:ARG:C	1:H:255:GLN:N	2.71	0.45
1:C:174:CYS:HB2	1:C:284:ARG:HG2	1.99	0.45
1:F:225:ASN:HB2	1:F:232:PHE:CE2	2.51	0.45
1:G:158:PHE:HB2	1:G:291:PRO:CD	2.46	0.45
1:D:184:TRP:HD1	1:D:220:TRP:CE3	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:HD1	1:B:220:TRP:CE3	2.34	0.44
1:C:259:CYS:SG	1:C:273:CYS:HB3	2.57	0.44
1:H:253:ARG:O	1:H:254:SER:CB	2.61	0.44
1:G:159:VAL:HG23	1:G:291:PRO:HG3	1.99	0.44
1:C:163:CYS:SG	1:C:174:CYS:SG	3.08	0.43
1:F:252:SER:HB2	1:F:254:SER:OG	2.18	0.43
1:H:184:TRP:HD1	1:H:220:TRP:CE3	2.36	0.43
1:H:254:SER:O	1:H:255:GLN:HB2	2.17	0.43
1:A:158:PHE:HD2	1:A:291:PRO:HD2	1.83	0.43
1:G:245:TRP:CH2	1:G:250:PRO:HB3	2.53	0.43
1:A:193:ASP:OD2	1:H:182:LYS:HA	2.19	0.43
1:D:263:ARG:HE	1:D:267:ARG:NH2	2.17	0.42
1:H:253:ARG:O	1:H:255:GLN:O	2.37	0.42
1:D:229:LYS:CE	1:F:254:SER:N	2.67	0.42
1:E:174:CYS:HB2	1:E:284:ARG:HG2	2.01	0.42
1:C:184:TRP:HD1	1:C:220:TRP:CE3	2.37	0.42
1:B:263:ARG:HE	1:B:267:ARG:NH2	2.18	0.42
1:H:201:ILE:HG12	1:H:210:LEU:HD13	2.01	0.42
1:D:226:LEU:CD2	1:D:233:ILE:HG13	2.50	0.41
1:G:260:VAL:HG22	1:G:270:ASP:HB3	2.02	0.41
1:A:158:PHE:HB2	1:A:291:PRO:CD	2.50	0.41
1:C:158:PHE:HB2	1:C:291:PRO:CD	2.50	0.41
1:D:228:LEU:O	1:D:229:LYS:HG3	2.21	0.41
1:F:224:ARG:O	1:F:232:PHE:HA	2.20	0.41
1:H:200:SER:HA	1:H:234:TRP:CE3	2.56	0.41
1:A:228:LEU:HD23	1:A:231:GLU:HB3	1.91	0.41
1:F:201:ILE:HG12	1:F:210:LEU:HD13	2.02	0.41
1:B:263:ARG:HH11	1:F:254:SER:HA	1.86	0.41
1:G:200:SER:HA	1:G:234:TRP:CE3	2.56	0.41
1:D:228:LEU:O	1:D:229:LYS:CG	2.69	0.41
1:F:223:LEU:HB3	1:F:260:VAL:HB	2.02	0.41
1:B:290:PRO:HA	1:B:291:PRO:HD3	1.89	0.40
1:C:158:PHE:HD2	1:C:291:PRO:HD2	1.86	0.40
1:G:201:ILE:HG12	1:G:210:LEU:HD13	2.03	0.40
1:G:225:ASN:OD1	1:G:230:GLY:O	2.38	0.40
1:F:200:SER:HA	1:F:234:TRP:CE3	2.56	0.40
1:B:200:SER:HA	1:B:234:TRP:CE3	2.56	0.40
1:C:163:CYS:HG	1:C:174:CYS:HG	1.51	0.40
1:H:255:GLN:C	1:H:257:GLU:H	2.25	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:NH1	1:H:254:SER:O[1_655]	1.69	0.51
1:A:267:ARG:CZ	1:H:254:SER:O[1_655]	1.81	0.39
1:A:267:ARG:NH2	1:H:254:SER:O[1_655]	1.83	0.37
1:G:231:GLU:OE1	1:H:251:THR:CG2[1_655]	2.06	0.14

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	129/143 (90%)	121 (94%)	8 (6%)	0	100	100
1	B	129/143 (90%)	120 (93%)	9 (7%)	0	100	100
1	C	128/143 (90%)	120 (94%)	8 (6%)	0	100	100
1	D	131/143 (92%)	120 (92%)	11 (8%)	0	100	100
1	E	126/143 (88%)	120 (95%)	6 (5%)	0	100	100
1	F	124/143 (87%)	114 (92%)	9 (7%)	1 (1%)	16	46
1	G	133/143 (93%)	121 (91%)	12 (9%)	0	100	100
1	H	127/143 (89%)	117 (92%)	10 (8%)	0	100	100
All	All	1027/1144 (90%)	953 (93%)	73 (7%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	161	ASN

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	114/120 (95%)	100 (88%)	14 (12%)	4	19
1	B	113/120 (94%)	101 (89%)	12 (11%)	6	24
1	C	113/120 (94%)	100 (88%)	13 (12%)	5	21
1	D	114/120 (95%)	104 (91%)	10 (9%)	9	31
1	E	111/120 (92%)	97 (87%)	14 (13%)	4	18
1	F	109/120 (91%)	101 (93%)	8 (7%)	13	38
1	G	115/120 (96%)	106 (92%)	9 (8%)	11	36
1	H	110/120 (92%)	102 (93%)	8 (7%)	13	38
All	All	899/960 (94%)	811 (90%)	88 (10%)	7	28

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	VAL
1	A	160	CYS
1	A	162	THR
1	A	195	GLU
1	A	224	ARG
1	A	226	LEU
1	A	227	ASP
1	A	228	LEU
1	A	231	GLU
1	A	241	ASP
1	A	261	MET
1	A	265	SER
1	A	273	CYS
1	A	289	THR
1	B	159	VAL
1	B	160	CYS
1	B	162	THR
1	B	165	GLU
1	B	195	GLU
1	B	224	ARG
1	B	241	ASP
1	B	261	MET
1	B	265	SER
1	B	273	CYS
1	B	285	LEU

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Mol	Chain	Res	Type
1	B	289	THR
1	C	159	VAL
1	C	160	CYS
1	C	162	THR
1	C	165	GLU
1	C	195	GLU
1	C	226	LEU
1	C	241	ASP
1	C	253	ARG
1	C	261	MET
1	C	263	ARG
1	C	265	SER
1	C	273	CYS
1	C	289	THR
1	D	159	VAL
1	D	160	CYS
1	D	162	THR
1	D	224	ARG
1	D	228	LEU
1	D	241	ASP
1	D	261	MET
1	D	265	SER
1	D	273	CYS
1	D	289	THR
1	E	160	CYS
1	E	162	THR
1	E	195	GLU
1	E	224	ARG
1	E	241	ASP
1	E	251	THR
1	E	252	SER
1	E	253	ARG
1	E	261	MET
1	E	265	SER
1	E	269	ASN
1	E	273	CYS
1	E	275	ARG
1	E	289	THR
1	F	192	ASP
1	F	195	GLU
1	F	197	GLN
1	F	241	ASP

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Mol	Chain	Res	Type
1	F	255	GLN
1	F	261	MET
1	F	273	CYS
1	F	282	CYS
1	G	159	VAL
1	G	160	CYS
1	G	165	GLU
1	G	195	GLU
1	G	241	ASP
1	G	261	MET
1	G	265	SER
1	G	273	CYS
1	G	289	THR
1	H	195	GLU
1	H	228	LEU
1	H	241	ASP
1	H	251	THR
1	H	254	SER
1	H	261	MET
1	H	265	SER
1	H	273	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	B	169	ASN
1	C	169	ASN
1	C	255	GLN
1	D	169	ASN
1	D	239	HIS
1	E	169	ASN
1	E	216	HIS
1	F	197	GLN
1	F	225	ASN
1	G	169	ASN
1	G	269	ASN
1	H	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	133/143 (93%)	0.47	5 (3%)	44	26	27, 49, 80, 98	0
1	B	133/143 (93%)	0.43	2 (1%)	72	52	28, 48, 84, 105	0
1	C	132/143 (92%)	0.62	8 (6%)	27	15	31, 50, 82, 96	0
1	D	133/143 (93%)	0.66	11 (8%)	17	10	35, 58, 87, 101	0
1	E	130/143 (90%)	0.58	10 (7%)	19	11	28, 49, 79, 108	0
1	F	128/143 (89%)	0.64	7 (5%)	30	17	35, 58, 85, 106	0
1	G	135/143 (94%)	0.64	6 (4%)	39	22	38, 57, 86, 98	0
1	H	129/143 (90%)	0.58	7 (5%)	31	18	32, 57, 90, 111	0
All	All	1053/1144 (92%)	0.58	56 (5%)	32	18	27, 54, 85, 111	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	216	HIS	3.8
1	A	227	ASP	3.6
1	F	193	ASP	3.6
1	F	251	THR	3.5
1	H	192	ASP	3.2
1	E	291	PRO	3.2
1	C	291	PRO	3.2
1	G	158	PHE	3.2
1	G	157	GLY	3.1
1	A	291	PRO	3.1
1	E	230	GLY	2.9
1	C	263	ARG	2.9
1	D	165	GLU	2.9
1	F	228	LEU	2.8
1	G	269	ASN	2.8
1	G	161	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	227	ASP	2.7
1	H	163	CYS	2.7
1	D	289	THR	2.7
1	G	291	PRO	2.6
1	D	273	CYS	2.6
1	H	160	CYS	2.6
1	C	217	THR	2.6
1	E	217	THR	2.6
1	E	255	GLN	2.5
1	B	253	ARG	2.5
1	D	162	THR	2.5
1	D	283	ASP	2.5
1	E	290	PRO	2.5
1	D	158	PHE	2.4
1	E	163	CYS	2.4
1	D	161	ASN	2.4
1	D	230	GLY	2.4
1	D	160	CYS	2.3
1	H	193	ASP	2.3
1	E	273	CYS	2.3
1	D	290	PRO	2.3
1	C	162	THR	2.3
1	F	255	GLN	2.2
1	A	165	GLU	2.2
1	E	270	ASP	2.2
1	F	208	ASP	2.2
1	H	208	ASP	2.2
1	C	251	THR	2.2
1	G	165	GLU	2.2
1	H	255	GLN	2.1
1	A	157	GLY	2.1
1	F	174	CYS	2.1
1	B	291	PRO	2.1
1	E	195	GLU	2.1
1	C	163	CYS	2.1
1	D	192	ASP	2.1
1	F	165	GLU	2.1
1	A	228	LEU	2.0
1	C	158	PHE	2.0
1	H	288	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.